

University of Groningen

## Reducing adsorption in nanochannels

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## **Abstract Book CHAINS 2016**

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# CHAINS 2016 General Information

## Wifi connection

Wifi is available during the entire conference in all rooms of the venue. This should allow basic wifi applications, such as browsing on the web and emailing in the entire conference center. For a high speed connection requiring a higher up and download capacity additional voucher can be purchased at the hotel desk.

## Travel instructions

### Shuttle busses

There will be a special bus service from Eindhoven Central station to CHAINS 2016 and back. At Eindhoven Central station please follow the signs 'UITGANG NOORD/BEURSGEBOUW'. Walk through the exit and directly go to the right. After approximately 25 metres you will find the buses at your right hand (around the corner).

### Arrival

On Tuesday & Wednesday morning the bus service will operate continuously between 08.00 hrs and 09.30 hrs. The estimated time travel to the venue is about 25 minutes.

After the meeting on Wednesday & Thursday a shuttle bus to Eindhoven central station will be available at the exit of the CHAINS venue (Beneluxfoyer). The buses will depart as of 17.30 to 18.00 (6 Dec) and 17.30-18.00 (7 Dec) from the Benelux Foyer (not the main entrance of the Koningshof!).

### Regular bus lines

If you want to leave during the programme you can use the regular public transport (bus lines 149 & 150) to the station. These buses leave at the main entrance of the Koningshof. Both buses will bring you to Eindhoven Station. This bus ride will take approximately 30 minutes.

### NH Geldrop

If you are staying at the NH Geldrop, the transfers to the NH Geldrop will be available on Wednesday evening between 22.00 and 01.00 hrs. On Thursday morning there will be one transfer at 08.00 o'clock.

## Drinks on Monday and Tuesday evening

In the evening you can get drinks at your own expense at the bars opened by de Koningshof. Please note that you cannot charge your purchases to your room number.

Coins will be available at the sales point near the Brabantthal.

## CHAINS APP

For all detailed and latest information about all presentations, sessions, speakers and participants, please download the CHAINS 2016 app in the App-store (Apple) or Google Play Store (Android). You can also schedule your personal programme and find your way to and at the venue.

## Social media



NWOCHAINS@2016chains  
#chains2016



[www.facebook.com/NWOCEW](http://www.facebook.com/NWOCEW)

CHAINS 2016 Programme  
Version date: 1 December 2016

Tuesday 6 Dec - day 1									
8.30 - 10.00	Registration and coffee, put up posters day 1/2: ST, SM, CSM, MM, C, CCHK, and PT								
10.00 - 10.10	Opening (Beneluxzaal)								
10.10 - 10.55	Plenary lecture: Clare Grey University of Cambridge (Beneluxzaal)  Following Function in Real Time: Structure and Dynamics In Batteries and Supercapacitors								
10.55 - 11.15	Coffee break								
Room	Room 55-57	Boszaal	Room 58	Parkzaal	Auditorium	Room 82/83	Room 63/64	Room 65	
	Photocatalysis and Solar Fuels Chair: Guido Mul	Cooperative ligand design Chair: Marc-Etienne Moret	Catalytic and Nano Engineering Chair: Leon Lefferts	Microscopy of Soft matter Chair: Frieder Mugele	Responsive Supramolecular Systems Chair: Nathalie Katsonis	Solar energy conversion Chair: Petra de Jongh	Theory development Chair: Luuk Visscher	Dynamics and reactions Chair: Joerg Meyer	
11.15 - 11.35	W. Vijselaar (UT; Huskens) Site-Selectively Patterned NiMo on Silicon Micropillars with Radial pn-Junction for Unprecedented Hydrogen Production	A.F. Orsino (UU; Moret) Synthesis and Reactivity of Nickel Complexes Bearing a Non- Innocent Diphosphine Ketone ligand	F. Grillo (TUD; Van Ommen) Controlled Growth of Metal Nanoparticles on Substrates via Scalable Atmospheric Pressure Atomic Layer Deposition	A. Aloï (TU/e; Voets) Imaging the topology of soft and deformable interfaces by single- molecule localization microscopy	A.H. Gelebart (TU/e; Schenning) Large amplitude light-driven motions in liquid crystal networks	J. Zuo (UvA; Zhang) New approach in constructing highly efficient near infrared light upconversion nanomaterials	K. Doblhoff-Dier (LEI; Kroes) Quantum Monte Carlo for transition metal containing dimers	J. Onvlee (RU; Groenenboom) Unraveling molecular Collisions	
11.35 - 11.55	I. Siretanu (UT; Mugele) In operando characterization of light-induced charge variations of photocatalytically active TiO2 surface by AFM	C. te Grotenhuis (UvA; De Bruin) Synthetic Applications of Cobalt(III)-Carbene Radicals	K.T. Coenen (TU/e; Gallucci) On the adsorption of CO2 and H2O on hydrotalcite-based sorbents	H. Friedrich (TU/e; Sommerdijk) Quantitative Multiscale Electron Microscopy of Functional Materials	G.M. ter Huurne (TU/e; Palmans) Supramolecular polymers from a different angle – The characteristics and limits of single- chain folding	W.M.J. Franssen (RU; Kentgens) Solid-state NMR study of perovskite bulk and thin films for solar cell applications	H. Zulfikri (UT; Filippi) Local multi-resonance description of electronic excited states in quantum Monte Carlo	P. Spiering (LEI; Meyer) Bond-breaking and making on metal surfaces – a breakdown of the Born-Oppenheimer approximation?	
11.55 - 12.15	J.H.J. Wijten (UU; Weckhuysen) Charge Carrier Behaviour in MOFs developed for Photocatalytic Applications	M.N. Devillard (UvA; Van der Vlugt) Versatile Reactivity and Catalysis of Lutidine-based Ligands with Transition Metal and Main Group Elements	R.W. Crisp (TUD; Houtepen) Synthesis and deposition of non- toxic, stable colloidal semiconductor nanocrystals for lighting and photovoltaic applications	L. Grebikova (UT; Vancso) Angle-dependent single chain adhesion of polymers by AFM	B. Kriete (RUG; Pchenitchnikov) Chemistry-Driven Supramolecular Architectures	G. Wang (UU; Ngene) Cu2O and CuS Nanoparticles: Preparation and Photocatalytic Performance	M.K. Wibowo (RUG; Broer) Nonorthogonal configuration interaction for calculating the singlet fission efficiency	Z. Sun (RU; Parker) REMPI spectroscopy of the carbon monoxide molecule	
12.15 - 12.25	Poster pitches 1. Rohit Chaudhary (TU/e) 2. Nazila Masoud (UU)	Poster pitches 1. Suzanne Jansze (EFPL)	Poster pitches 1. Nathan Straathof (TU/e) 2. Liang Lin (TU/e) 3. Maria Ronda Lloret (UvA)	Poster pitches 1. Serhil Mytnyk (TUD) 2. Olessya Loiko (TU/e) 3. Frankje de Boer (UU)	Poster pitches 1. Digvijay Gahtory (WUR) 2. Stijn Kragt (TU/e) 3. Hongbo Yuan (RU)	Poster pitches 1. Rochan Sinha (DIFFER) 2. Maria Gélvez-Rueda (TUD) 3. Yihui Zhao (DIFFER)	Poster pitches 1. Felipe Zapata (VU) 2. Marwa Farag (RUG) 3. Mark Koenis (UvA)	Poster pitches 1. Damla Inan (TUD) 2. Merijn Blaakmeer (RU) 3. Xueqing Zhang (DIFFER)	
12.25 - 14.00	Lunch & poster session 'odd' for ST, SM, CSM, MM, C, CCHK, and PT posters								
Room	Boszaal		Auditorium		Room 58		Room 63/64		
Themed sessions	X-ray experiments of Materials and Catalysis Chair: Frank de Groot		Chemistry at the nanoscale Chair: Joost Reek		Process Intensification and Flow Chemistry - 1 Chair: Andrzej Stankiewicz		Molecular Assemblies Chair: Albert Schenning		
14.00 - 14.30	Florian Meirer (UU) X-ray microscopy at multiple length scales – the showcase of metal poisoning of catalyst particles		Wesley Browne (RUG)		Martin van Sint-Annaland (TU/e) Fluidised bed membrane reactors for ultra-pure H2 production		Tom de Greef (TU/e) System-level Investigations of one-dimensional self- assembly		
14.30 - 14.50	Moniek Tromp (UvA) The active site in the spotlight!		S. Gonell (UvA; Reek) Catalysis at extremely high local concentrations by catalyst confinement in M12L24 nano-cages		M. Escriba-Gelonch (TU/e; Hessel) Continuous processing of Vitamin D3 with integrated high-T photo flow chemistry and antisolvent crystallization		N. Tiwari (TU/e; Van der Schoot) Mixing kinetics of reversible copolymerization		
14.50 - 15.10	Jan-Philip Hoffman (TU/e) Synchrotron-based X-ray Structural Analysis of Functional Materials Towards Catalytic Structure- Performance Relationships		S.J. Wezenberg (RUG) Allosteric regulation of the rotational speed in light- driven molecular motors		M.A. Reus (TUD; Stankiewicz) Crystallization in composite hydrogels for controlling polymorphism		I. Kryven (UvA; Bolhuis) Multilayer approach to modelling of interconnected soft matter structures		
15.10 - 16.00	Coffee break & Poster session 'odd' for ST, SM, CSM, MM, C, CCHK, and PT posters (continued)								
Room	Room 55-57	Boszaal	Room 58	Parkzaal	Auditorium	Room 82/83	Room 63/64	Room 65	
	Zeolites for catalysis Chair: Evgeny Pidko	Tranformations with Grignard reagents Chair: Tatí Fernández-Ibáñez	Process Intensification and Flow Chemistry - 2 Chair: Volker Hessel	Colloids Chair: Willem Kegel	Polymer Materials Chair: Rint Sijbesma	2-Dimensional Nanomaterials Chair: Gregory Schneider	Light harvesting Chair: Francesco Buda	Spectroscopy tracking of reactions Chair: Jos Oomens	
16.00 - 16.20	I. Yarulina (TUD; Kapteijn) Synergetic Effect of Lewis and Brønsted Acidity in Methanol to Olefins Reaction	F. Lanza (RUG; Harutyunyan) Catalytic asymmetric synthesis of chiral N-heterocyclic aromatic compounds	S. Susanti (RUG; Yue) Continuous chiral separations in microreactors	V. Meester (LEI; Kraft) Colloidal recycling: Reconfiguration of Random Aggregates into Patchy Particles	S. Kommeren (TU/e; Bastiaansen) Structured amphiphilic and omniphobic materials for antifouling applications	P.H. Jacobse (UU; Klein Gebbink) Nanographenes from (halo)bianthryls on Cu(111) and Au(111)	P. López-Tarifa (VU; Visscher) An Ab-initio Study of the Spectroscopic Properties of Solubilized LHCII	L.J.M. Kempkes (RU; Oomens) Deamidation reactions of asparagine and glutamine containing peptides investigated by ion spectroscopy	
16.20 - 16.40	N. Kosinov (TU/e; Hensen) Stable performance of Mo/HZSM-5 in methane aromatization	J.E. Borger (VU; Lammertsma) Functionalization of P4 Using Lewis Acid Stabilized Bicyclo[1.1.0]tetraphosphabutane Anions	D.J.G.P. van Osch (TU/e; Tuinier) Removal of Metal Ions from Water with Hydrophobic Deep Eutectic Solvents	F. Hagemans (UU; Imhof) Sculpting silica colloids by etching silica rods with non-uniform compositions	M. Fernandez Castano-Romera (TU/e; Sijbesma) Strain-stiffening in synthetic hydrogels: Mimicking biological networks	V.B. Tran (RUG; Stöhr) Self-assembly and on-surface polymerization of bromine- functionalized pyrene derivatives on noble metal surfaces	K.M. Felter (TUD; Grozema) Long-range exciton diffusion in perylene diimides mediated by singlet fission	A.M. De Carvalho Vicente Da Cunha (RUG; Jansen) Benchmarking simulation protocols for the amide I spectra of proteins	
16.40 - 17.00	R.Y. Rohling (TU/e; Pidko) Novel molecular recognition and confinement-driven reactivity concepts in zeolite catalysis for biomass valorization	X. Yan (RUG; Harutyunyan) Chiral amides via catalytic asymmetric synthesis	F. Khodadadian (TUD, Stankiewicz) Modeling an annular LED-based photocatalytic reactor for gas phase applications	A. Gonzalez Garcia (TU/e; Tuinier) Tuning the phase diagram of colloid-polymer mixtures via additional soft colloidal interactions	J. Xu (RUG; Loos) Polymer-templated chemical solution deposition of ordered multiferroic nanocomposites	A. Pustovarenko (TUD; Gascon) Surfactant assisted synthesis of metal organic framework nanosheets. Applications in gas separation and chemical sensing	R. Alessandri (RUG; Broer) In silico characterization of polymer-fullerene organic photovoltaic bulk heterojunctions	M. Caldarola (LEI; Orrit) Single-molecule redox reaction detection by enhanced fluorescence	
17.00 - 17.35	Snack break								
Room	Room 55-57	Boszaal	Room 58	Parkzaal	Auditorium	Room 82/83	Room 80/81	Room 63/64	Room 65
	Fischer-Tropsch Catalysis Chair: Ivo Filot	Water oxidation Chair: Dennis Hetterscheid	Modelling of processes Chair: Sascha Kersten	Self-assembly Chair: Andrei V. Petukhov	Biobased Chemistry Chair: Katja Loos	Molecular Materials Chair: Leo Jenneskens	Inorganic nanoparticles Chair: Celso de Mello Donega	Multiscale modeling Chair: Claudia Filippi	Fast spectroscopy Chair: Michel Orrit
17.35 - 17.55	S. Kanungo (TU/e; Neira D'Angelo) Gas phase propene epoxidation on gold: Catalyst design and mechanistic insight	C.J.M. van der Ham (LEI; Hetterscheid) In operando studies on molecular water oxidation catalysts	R. Westerhof (UT; Kersten) Effects of mass transfer and alkaline metals on the pyrolysis of cellulose	S. Ouhajji (UU; Petukhov) Multiscale self-assembly of microtubes	F. van der Kils (WUR; Bitter) Structure-property relations of biobased polyesters from 1,4- butanediol-analogues and biobased diacids	J.B. ten Hove (WUR; Velders) Supramolecular Nano- Assemblies for Biomedical Diagnostic Applications	E.J. van Harten (UU; Meijerink) InP-based quantum dots: A good cadmium-free alternative?	J.M. Boereboom (UU; Bulo) Adaptive QM/MM: Current Limitations and Advances	Y. Zhang (UvA; Brouwer) Extreme ultraviolet photoreactions of tin oxo cages
17.55 - 18.15	C. Hernández Mejía (UU; Zecevic) Porosity enhancement of niobia-supported cobalt catalysts for Fischer–Tropsch Synthesis	S.K. Padamati (RUG; Browne) Solvent dependence of the formation of reactive non- heme intermediates with H2O2	S. Das (TU/e; Kuipers) DNS for flow and heat transfer through random open-cell solid foams: Development of an IBM based CFD model	D. Wang (UU; Van Blaaderen) Self-assembled Supraparticles by Spherical Confinement	T.G. Meinds (RUG; Heeres) Bio-based building block for polymer synthesis using advanced oxidation systems	W. Noteborn (LEI; Kieltyka) Self-assembly pathway modulation of a low molecular weight hydrogelator using polymeric crosslinkers	M. van der Linden (UU; De Groot) Unravelling the synthesis mechanism of ligand- protected silver nanoclusters	A. Tiwari (UvA; Ensing) Reactive trajectories of the Ru2+/3+ electron transfer reaction and the connection to Marcus' theory	J.D. Lauth (TUD; Siebbeles) Ultrafast Dynamics of Electron Hole Pairs in Ultrathin 2D InSe Layers
18.15 - 18.35	M.J. Louwerse (UU; De Jong) Progress in understanding iron based Fischer-Tropsch catalysis for olefin synthesis	J.M. de Ruiter (LEI; Buda) A closed system approach to investigate the catalytic cycle of a copper water oxidation catalyst	L.A. Truter (TU/e; Neira D'Angelo) Development of a continuous process for hydrothermal conversion of lignin	Y. Guo (UU; Kegel) Reversible encapsulation of large colloids by oppositely charged small colloids	H.C. Genuino (UU; Bruijninx) A New Tandem Catalytic Route to Renewable Aromatic Chemicals from Biobased Furans	E.B. Reijers (UU; Jenneskens) Degradation and Preservation of Contemporary Photo-Works	M.T. Hembury (UU; Vermonden) Gold quantum dot-decorated micelles for multimodal imaging and therapy	K.M. Visscher (VU; Geerke) A systematic approach to calibrate a transferable force field parameter set	M. Klotz (VU; Kennis) Spectral Watermarking in Femtosecond Stimulated Raman spectroscopy: resolving the nature of the carotenoid S* state
18.35 - 18.45	Poster pitches 1. Tilde Pellegrini (RUG) 2. Andrea Gheorge (UvA)	No poster pitches	No poster pitches	Poster pitches 1. Pim Frederix 2. Mark van Rijt 3. Vasudevan Lakshminarayanan	Poster pitches 1. Beatrice Adelizzi (TU/e) 2. Huey Wen Ooi (UM) 3. Zino Leijten(TU/e)	Poster pitches 1. Ester van Andel (WUR) 2. Xue Liu (LEI) 3. Jody Lugger (TU/e)	Poster pitches 1. Giulia Mirabello (TU/e) 2. Matteo Parente (DIFFER) 3. Karthikeyan Gnanasekaran (TU/e)	Poster pitches 1. Jurn Heinen (UvA) 2. Selim Sami (RUG)	Poster pitches 1. Dina Petrova (UvA) 2. Sandra Wiersma (UvA) 3. Gianluca Grimaldi (TUD)
18.45 - 20.00	Dinner								
20.00 - 22.00	Poster Session 'even' for ST, SM, CSM, MM, C, CCHK, and PT posters							21.00 - 22.00 Meeting group leaders	
22.00 - 01.00	Evening Programme							22.00 - 23.00 KNCV Pub Quiz	

Catalysis

Process Technology

Materials Chemistry

Physical & Theoretical Chemistry

Wednesday 7 Dec - day 2										
7.00 - 8.30	Breakfast									
8.30 - 9.00	Keynote: Wybren Jan Buma University of Amsterdam (Room 82/83)  High-resolution laser spectroscopy of photoactive materials: light on the dark side of the force			Keynote: IJla Voets Eindhoven University of Technology (Auditorium)  Hot proteins on cool crystals: crystal growth modulation by ice-binding proteins			Keynote: Joost Reek University of Amsterdam (Room 63/64)  Catalysis in self-assembled confined spaces: Control of catalyst properties by the second coordination sphere			
Room	Room 55-57	Room 58	Room 65	Parkzaal	Auditorium	Room 82/83	Room 80/81	Room 63/64	Boszaal	
	Catalytic organic synthesis Chair: Jarl Ivar van der Vlugt	Proton reduction catalysis Chair: Lies Bouwman	Glasses Chair: Arnout Imhof	Protein-peptides Chair: Mireille Claessens	Catalysis Chair: Hong Zhang	Molecular crystals Chair: Herma Cuppen	Electrochemistry Chair: Klaus Mathwig	NMR Spectroscopy Chair: Arno Kentgens	Astrochemistry Chair: Harold Linnartz	
9.05 - 9.25	F. Trausel (TUD; Eelkema) Activation of an organocatalyst by a chemical signal	R. Becker (UvA; Woutersen) An [FeFe]-hydrogenase mimic with an electron reservoir for efficient proton reduction in aqueous media	R. Higler (WUR; Van der Gucht) Vitrification as a dynamical connectivity transition	S. Lindhoud (UT; Claessens) Proteins in complex coacervates	J.E. van den Reijen (UU; De Jongh) Supported Silver Catalysts for Ethylene Epoxidation	M. Smets (RU; Cuppen) Understanding the solid-state phase transitions in molecular crystals	H.A.A. Al-Kutubi (RUG; Mathwig) Reducing adsorption in nanochannels: from fundamental understanding to practical application	J.O. Brauckmann (RU; Van Eck) MicroMAS NMR - Enhanced Resolution and Sensitivity combining Homonuclear Decoupling and Inverse Detection	T.A. Hamlin (VU; Bickelhaupt) B-DNA Stability and Replication in Non-Terran Bio-Solvents	
9.25 - 9.45	E. Romero (RUG; Fraaije) Discovery and engineering of robust Baeyer-Villiger monooxygenases	S. Luo (LEI; Bouwman) Syntheses, Structures, and Electrocatalytic Hydrogen Production of N-Functionalized Ni-NHC Complexes	J. M. van Doorn (WUR; Sprakel) Linking particle dynamics to local connectivity in colloidal gels	D.C. Schoenmakers (RU; Kouwer) Site-selective crosslinking of biomimetic hydrogels: Tuning gel mechanics without changing the architecture	M.E.Z. Velthoen (UU; Weckhuysen) UV-Vis/DFT Study on Activation of Zirconocene Species in Zr/MAO/SiO2 Polymerization Catalysts	A.H.J. Engwerda (RU; Vlieg) Attrition enhanced deracemization of chiral sulfoxides	A. Longo (NWO; Bras) In situ spectroelectrochemical study of Ni-Bi and NIOOH OECs	F. Azadi (LEI; Pandit) In situ probed solid-state NMR on photosynthetic thylakoid membranes	K. Doney (LEI; Linnartz) High resolution IR spectroscopy of hydrocarbon radicals of astrophysical interest	
09.45 - 10.00	Coffee break registration participants day 2/3, put up odd & even posters of day 2/3: PR, NA, LB, BMC, DS, SR, MC and AC									
10.00 - 10.15	Opening Plenary day (Beneluxzaal)									
10.15 - 11.00	Plenary Lecture: Odile Eisenstein University of Montpellier (Beneluxzaal)  Computational chemistry from Reactivity to NMR calculations									
11.00 - 11.30	KNCV Gold Medal Lecture: Syuzanna Harutyunyan University of Groningen (Beneluxzaal)  Catalytic enantioselective synthesis of functional molecules: control over selectivity and reactivity									
11.30 - 12.15	Plenary Lecture: Sarah Reisman California Institute of Technology (Beneluxzaal)  Necessity is the Mother of Invention: Natural Products and the Chemistry they Inspire									
12.15 - 14.00	Lunch 12.15-14.00: Networking lunch (separate registration needed) , room Uithof 12.30-13.30: DUBBLE session, room 55-57 13.20-13.50: Lecture by our sponsor: VO Patents on 'Patents and Funding', room 58 13:30-14:00: Q&A session ARC CBBC, room 21									
Room	Room 80/81	Room 63/64	Parkzaal	Auditorium	Room 82/83	Boszaal	Room 55-57	Room 58	Room 52	Room 65
Focus sessions	Activity-based protein profiling creates novel opportunities in drug discovery  Chair: Kim Bonger	Dynamics and kinetics of reactive and scattering processes  Chairs: Geert-Jan Kroes & Herma Cuppen	Bio-Inspired Chemistry: Nature as a source of inspiration in chemistry  Chair: Bert Klein Gebbink	Self-organization at Interfaces: from controllable interactions to 2D materials  Chair: Daniel Vanmaekelbergh	Molecular organization and function of chromatin  Chair: Hugo van Ingen	Industry-meets-Science Molecular biosensors  Chair: Menno Prins	Industry-meets-Science Stimuli-Responsive Materials  Chair: Maarten Smulders	Industry-meets-Science Continuous flow catalysis  Chair: Floris Rutjes	Organized by KNCV Chemical entrepreneurship (startup and scale up)  Chair: Peter van Tilburg	Organized by KNCV Chemistry Education in the Netherlands  Chair: Jeroen Cornelissen
14.00 - 15.20	1. Ed Tate (Imperial College) 2. Paul Geurink (LUMC; Ovaa) Diubiquitin FRET probes to quantify ubiquitin linkage specificity of deubiquitinases 3. Martijn Verdoes (RUMC) Quenched fluorescent cysteine cathepsin probes: tumor imaging and immunotherapy 4. Hui Deng (LEI; Van der Stelt) Discovery of Chemical Probes to Study Brain Lipid Signaling	1. Rainer Beck (EPFL, Switzerland) Exploring Gas/Surface Reaction Dynamics via Quantum State Resolved Molecular Beam Experiments 2. Davide Miglierini (LEI; Kroes) Accurate simulation of a polyatomic molecule-metal surface reaction: dissociative chemisorption of CHD3 on Pt(111) and Ni(111) 3. Adrien Fredon (RU; Cuppen) Admolecules mobility on interstellar icy dust particles 4. Ganna Shchygol (SCM; Goumans) Modeling reactions with ReaxFF in MOFs with defects	1. Jan van Esch (TUD) 2. Pradip Ghosh (UU; Klein Gebbink) Proton and electron responsive β-diiminates: studies of redox activities in transition metal complexes 3. Wilhelm Huck (RU) The end of chemistry... the beginning of life	1. Jaco J. Geuchlies (UU; Swart) Watching the birth of a nanocrystal Superlattice 2. René van Roij (UU) Self-organization by capillary interactions: the effect of interfacial curvature 4. Peter J. Beltramo (ETH Zurich) Self-assembly at fluid-fluid interfaces	1. Sjaak Neefjes (LUMC) Identifying old anti-cancer drugs as new epigenetic modifiers: the anthracyclines 2. Orkide Ordu (TUD; Dekker) Investigating the handedness dynamics of tetrasomes 3. Elzo de Wit (NKI) The cohesin release factor WAPL controls chromatin loop extension 4. Abdenour Soufi (Univ. of Edinborough) Mechanistic Insights Into Cell Fate Conversion	1. Jack van den Eerenbeemd (Phillips) The Effect of Reagents on the Performance of the Minicare 120 Point-of-Care System 2. Kristian Göeken (UT, Subramaniam) Localized surface plasmon biosensor 3. Thomas Cremers (Brains On-Line) Enzyme-based in-vivo biosensing of neurotransmitters and metabolites 4. Stefano Cappelli (TU/e, Prins) Biosensing based on particles and single-molecule methods for continuous monitoring	1. Filip Du Prez (Ghent University) Vitrimers: Recyclable Materials of the Future? 2. Rolf van Benthem (DSM) Macromolecular architectures at DSM: polymer templated silication technologies for antireflective coatings 3. Zeger Vroon (TNO) Window of the future (IR regulating windows)	1. Jesus Alcazar (Janssen-Cilag) Flow Chemistry as a Tool for Drug Discovery 2. Hannes P. L. Gemoets (TU/e, Noël) C-H functionalization in continuous flow 3. Daniel Blanco Ania (RU, Rutjes) Expanding the Applications of Flow Chemistry: Heterogeneous Catalysis and Large-Scale Photochemistry □	1. Ton Vries (Syncom) Syncom, how changing markets bring new business opportunities 2. Marcel Oogink (Duplaco) 3. Tjeerd Barf (Acerta Pharma) How (not) to start a biotech: From Dismissal to Deal 4. Peter van Tilburg (Enzyep)	1. Geert Hurenkamp (K.S.G. De Breul Zeist/Rodenborch-College Rosmalen) Excellence promoting educational materials 2. Joris van Elferen (Mondial College Nijmegen) Create your own education! 3. Petra Bouten (Summa Laboratorium, Eindhoven) New curriculum MBO
15.20 - 15.45	Coffee break									
15.45 - 15.55	Award ceremonies Top Sector Chemistry Student competition and Athena award									
15.55 - 16.40	Plenary Lecture: Jillian Buriak University of Alberta (Beneluxzaal)  Nanoscience Lives Here: Molecules, Materials, & Mechanisms									
16.40 - 17.25	Plenary Lecture: Jane Clarke University of Cambridge (Beneluxzaal)  Mechanistic studies of Folding upon Binding: Using Physics and Chemistry to Understand Biology									
17.25 - 17.35	Award ceremony 'start-up of the year' (Gouden KIEM) and announcement poster prizes day 1/2; Closing plenary day									
17.35 - 19.25	Dinner									
Room	Room 55-57	Room 58	Boszaal	Room 63/64	Parkzaal	Auditorium	Room 82/83	Room 80/81	Room 65	
	Analytical Tools I Chair: Maarten Honing	Mechanism of chemical reactions Chair: to be announced	Multicomponent Reactions Chair: Eelco Ruijter	Backer lecture Chair: Gerard Roelfes	Applied microbial mechanisms Chair: Kristina Djanashvili	Fluorescent sensors and imaging Chair: Maarten Merkkx	NMR methods Chair: Stefan Rudiger	(Prote)omics Chair: Tobias Dansen	Transcriptional regulation Chair: Fred van Leeuwen	
19.25 - 19.45	B. van Meerten (RU; Van Bentum) Overhauser Dynamic Nuclear Polarization for high sensitivity NMR in supercritical CO <sub>2</sub>	J. Nitsch (VU; Bickelhaupt) Bite-angle bending as key for understanding metal reactivity of d <sup>10</sup> _[M(NHC) <sub>2</sub> ] complexes	J.M. Saya (VU; Ruijter) Stereoselective one-step synthesis of complex alkaloid mimics by an interrupted Ugi cascade reaction	Masimo Giannerini (Janssen Pharmaceuticals, Inc.)  Advancing selectivity control with highly reactive organometallic reagents	D.Z. Sousa (WUR; Stams) Syngas fermentation by synthetic co-cultures of anaerobic microorganisms	M. Mastop (UvA; Goedhart) Novel fluorescent proteins applied in multiplexing of FRET sensors	M. Lescanne (LEI; Ubbink) Protein assignment using paramagnetic effects with PARAssign	M.E. Kamp (RUG; Van Haastert) A proteomic approach for identifying new key components of the chemotaxis signaling pathway	J. Rougeot (RUMC; Kamminga) Ezh2 is not essential for early embryonic development but is required for tissue maintenance in zebrafish	
19.45 - 20.05	B.W.J. Pirok (UvA; Peters) Making Analytically Incompatible Approaches Compatible	D. Zheng (UvA; Brouwer) Fluorescent cinchona alkaloids for single molecule studies of organocatalysis	V. Estevez Closas (VU; Orru) Exploiting Isocyanide-based multicomponent reactions in the design of small-molecule libraries		R. Medici (TUD; Hanefeld) Assessing diol dehydratase from Lactobacillus brevis for 2-butanone production	R. Arts (TU/e; Merkkx) Engineering bioluminescent sensor proteins for smartphone-based antibody diagnostics	D. Mance (UU; Baldus) Novel high-sensitivity approaches for in-situ NMR	L. van Dam (UMCU; Dansen) Quantitative Mass Spectrometry to identify targets of Peroxiredoxin dependent Redox Signaling	S. Schuster (RUMC; Van Rij) Using CRISPR/Cas9 to unravel the role of mammalian RNAi in antiviral immunity	
20.05 - 20.15	Poster pitches 1. Fleur van Beek (UvA) 2. Mengyun Xu (RUG)	Poster pitches 1. Sjors Wijnands (TU/e) 2. Liliana Cozzoli (RUG) 3. Shengqi Xiang (UU)	Poster pitches 1. Mira Holzheimer (RUG) 2. Pablo Ortiz (RUG) 3. Alejandra Riesco-Dominguez (RU)	Poster pitches 1. Tjerk Sminia (WUR) 2. Andrea Leoncini (UT) 3. Hidde Elferink (RU)	Poster pitches 1. Lara Villarino Palmaz (RUG) 2. Xin Chen (RUG) 3. Hanna Busch (TUD)	Poster pitches 1. Srividya Ganapathy (LEI) 2. Jan Pille (RU) 3. Patricia Alvarez Siero (RUG)	Poster pitches 1. Ingy Abdallah (RUG) 2. Cunliang Geng (UU)	Poster pitches 1. Can Araman (LEI) 2. Marcel van Willigen (UU) 3. Luca Ferrari (UU)	Poster pitches 1. Clemens Mayer (RUG)	
20.15 - 22.00	Poster Session 'odd' for PR, NA, LB, BMC, DS, SR, MC and AC posters							21.00 - 22.00 Meeting group leaders		
22.00 - 01.00	Evening Programme							22.00 - 23.00 KNCV Pub Quiz		
	Catalysis Analytical Chemistry		Process Technology (Bio-)Organic chemistry		Materials Chemistry Medicinal Chemistry		Physical & Theoretical Chemistry Biochemistry & Molecular Biology			

Catalysis	Process Technology	Materials Chemistry	Physical & Theoretical Chemistry
Analytical Chemistry	(Bio-)Organic chemistry	Medicinal Chemistry	Biochemistry & Molecular Biology



	Thursday 8 Dec - day 3								
7.00 - 8.30	Breakfast								
8.30 - 9.00	Keynote: Jan van Hest Eindhoven University of Technology (Auditorium)  Building life-like systems: artificial cells and organelles			Keynote: Peter Schoenmakers University of Amsterdam (Room 63/64)  Separation Technology for a Million Peaks (STAMP)			Keynote: Tjeerd Barf Acerta Pharma (Room 82/83)  Covalent Kinase Inhibition as A Versatile Approach in Drug Discovery		
Room	Room 55-57	Boszaal	Room 63/64	Room 58	Parkzaal	Auditorium	Room 82/83	Room 80/81	Room 65
	Hyphenated - MS Analysis Chair: Rawi Ramautar	Supramolecular Chemistry I Chair: Jan van Esch	Chemistry controlled with light Chair: Fred Brouwer	Anticancer drug approaches Chair: Frank Dekker	Photochemistry and Photoresponsive molecules Chair: Timothy Noel	Lipids as Tools Chair: Alexander Kros	Protein structure I Chair: Robbie Joosten	Membrane Proteins Chair: Albert Guskov	RNA Biology Chair: Ronald van Rij
9.05 - 9.25	K. Stavenhagen (LUMC, Wuhrer) In-depth Site-Specific N- and O-Glycosylation Analysis of Human C1-Inhibitor by C18-PGC-LC-MS/MS	S.C.C. van der Lubbe (VU; Fonseca Guerra) Multiply hydrogen-bonded arrays from a quantum chemical perspective	F. Lancia (UT; Katsonis) Muscle-like responses in light-driven polymer springs	L.N. Lameijer (LEI; Bonnet) L- versus D-glucose: targeting mitochondria with water-soluble photoactivatable ruthenium-based anticancer prodrug	W. Zhang (TUD; Arends) A 'Combinatorial Explosion' of Products through Photo-Chemo-Enzymatic Cascades	S. Scheidelaar (UU; Killian) Lipid membrane solubilization and nanodisc formation by the styrene maleic acid (SMA) co-polymer	B. van Beusekom (NKI; Joosten) Better protein structure models with homology-based hydrogen bond restraints	A. Stetsenko (RUG; Guskov) Mechanism of zinc transport in bacteria	J.P. Gerlach (RUMC; Mulder) Quantitative analysis of gene and protein expression in single-cells
9.25 - 9.45	B.M. Ziętek (VU; Kool) Nanofractionation analytics with parallel mass spectrometry for identification of cytochrome P4501A2 inhibitors in metabolic mixtures	S.J. Spa (LEI; Van Leeuwen) Orthogonal Functionalization of Ferritin via Supramolecular Re-Assembly	J. Escorihuela (WUR; Smulders) Rapid surface functionalization of hydrogen-terminated silicon by alkyl silanols	A. Geersing (RUG; Roelfes) Understanding the Mechanisms of Action of the Synthetic Bleomycin Mimic N <sub>4</sub> Py in Human Cell Cultures	M.M. Lerch (RUG; Feringa) Emerging Photoswitches for Functional Systems	L.M.C. Lima (LEI; Schneider) Lipids: a tool for graphene bionanotechnology	M. Wawrzyniuk (UU; Rudiger) Disordered proteins in the eyes of a molecular chaperone	S. Rempel (RUG; Slotboom) Membrane transporters for Vitamin B12: small proteins handling enormous molecules	C.C. Posthuma (LUMC; Snijder) Cyclophilin inhibitors cyclosporin A and Alisporivir block the replication of a broad range of nidoviruses
9.45 - 10.05	E. Dominguez-Vega (VU; Somsen) Probing protein heterogeneity, conformation and affinity by combining native capillary electrophoresis with MS and SPR	B. Bartolec (RUG; Otto) Towards Self-Replicating Molecules Forming Compartments	R.M. Putri (UT; Katsonis) Developing a bacterial semi-organelle into photo-responsive protein systems	M.J. van Haren (UU; Martin) Potent Inhibitors of Protein arginine N-methyltransferase designed to occupy both substrate binding sites	C. Bottecchia (TU/e; Noël) Development of batch and flow visible light photocatalytic methodology for application in chemical biology	A. Soler Canton (TUD; Danelon) Therapeutic liposome nanofactory	L. Xue (UU; Bonvin) Template-based protein-protein docking exploiting pairwise interfacial residues restraints	S. Ganapathy (LEI; De Grip) Towards the adaptation of rhodopsin proton-pumps using retinal analogs and directed evolution	M. Derksen (RUMC; Pruijn) Towards an RNase MRP activity assay
10.05 - 10.15	Poster pitches 1. Guilia Lambiase (VU) 2. Karlijn Bezemer (UvA)	Poster pitches 1. Pim de Vink (TU/e) 2. Selma Eising (RU) 3. Dowine de Bruijn (RUG)	Poster pitches 1. Mark Hoorens (UMCG) 2. Marjolein Soethoudt (LEI) 3. Xavier Gomez-Santacana (VU)	Poster pitches 1. Ingrid 't Hart (UU) 2. Raimond Heukers (VU)	Poster pitches 1. Aleksandr Pogodaev (RU) 2. Elliot Mock (LEI) 3. Alberto Juan Ruiz del Valle (UT)	Poster pitches 1. Hetty Manenschijn (Univ Geneva) 2. Amin Abolghassemi Fakhree (UT) 3. Lukasz Syga (RUG)	Poster pitches 1. Matti Pronker (UU) 2. Doreth Kok (NKI)	Poster pitches 1. Hendrik Sikkema (RUG) 2. Emanuela Crisafi (LEI) 3. Rajkumar Singh (RUG)	Poster pitches 1. Jeroen Strating (UU)
10.15 - 11.05	Coffee break & Poster session 'even' for PR, NA, LB, BMC, DS, SR, MC and AC posters								
Room	Room 55-57	Boszaal	Room 63/64	Room 58	Parkzaal	Auditorium	Room 82/83	Room 80/81	Room 65
	Analytical Tools II Chair: Louis de Smet	Analytical applications in life sciences Chair: Arjan Mank	Synthetic Methodology Chair: Jan van Maarseveen	Enzymology I Chair: Nathaniel Martin	Supramolecular Chemistry II Chair: Dennis Lowik	Biomembranes & Transport Chair: Dirk Slotboom	Chemical Biology I Chair: Cella Berkers	Protein regulation and networks Chair: Marjolein Kikkert	DNA structure and integrity Chair: Martijn Luijsterburg
11.05 - 11.25	N.N. Hamidon (RUG; Verpoorte) Enhanced flow control in easily fabricated paper-microfluidic devices	J. Yan (TU/e; Prins) Protein corona on nanoparticles analyzed by molecular barcodes	D. Heijnen (RUG; Feringa) Fast Cross-Coupling Reactions with Organolithium Reagents	H. Wapenaar (RUG; Dekker) Challenges in targeting bi-substrate enzymes: A histone acetyltransferase KAT8 case story	S. van Dun (TU/e; Milroy) Towards synthetic supramolecular intracellular signalling events using self-assembling bipyridine-discotic amphiphiles	X. Bao (UU; De Kroon) Yeast devoid of the essential membrane lipid phosphatidylcholine	V. Horn (LEI; Van Ingen) Employing peptide-based nucleosome-mimics to dissect the epigenetic read-out of H3K36me3	R.C.M. Knaap (LEI; Kikkert) Targeting the Middle-East respiratory syndrome coronavirus papain-like protease	A. Zelensky (EMC; Kanaar) Insertional mutagenesis: Uncovering a novel cellular mechanism of response to extremely low dose ionizing radiation
11.25 - 11.45	B. Wouters (UvA; Schoenmakers) Immobilized enzyme reactors in analytical chemistry	R. Penning (UU; Altelaar) In-depth pulsed SILAC/AHA labeling and phosphoproteomics study of the molecular events underlying mGluR-LTD	T. Krachko (VU; Slootweg) Unprecedented phosphinidene transfer reactions from carbene-phosphinidene adducts	A.P.A. Janssen (LEI; Van der Stelt) Chemoproteomic profiling of the serine hydrolase interaction landscape of the fatal drug BIA 10-2474	L. Schoonen (RU; Van Hest) Self-assembled nanoreactors based on the cowpea chlorotic mottle virus capsid	S. Koch (RUG; Driessen) Lipids activate SecA for high affinity binding to the translocon	E.A. Zaal (UU; Berkers) Targeting metabolic resistance to proteasome inhibitor therapy	S.A.G. Cuijpers (LEI; Vertegaal) Revealing an essential role for SUMO in cell cycle progression	M. Simonetta (NKI; Jacobs) DNA repair pathway choice: small MAD2L2 decides between giants 53BP1 and BRCA1
11.45 - 12.05	A. Astefanei (UvA; Cortals) Surface acoustic wave MS: extremely fast highly sensitive molecular analysis	J.C. Schoeman (LEI; Hankemeier) Cord blood metabolomics, studying in utero HIV-cART exposure in uninfected infants compared to controls	K. Naksomboon (UvA; Fernández-Ibáñez) Bidentate Ligands-Promoted Palladium-Catalyzed C-H Functionalization	V.R. Jumde (RUG; Hirsch) Design and Synthesis of Bioisosteres of Acylhydrazones as Stable Inhibitors of the Aspartic Protease Endothiapepsin	A. den Hamer (TU/e; Brunsveld) Supramolecular signalling platforms: 14-3-3 proteins as a scaffold	I. Faustino (RUG; Marrink) Insights on the transport mechanism of energy-coupling factor transporters using multiscale molecular dynamics simulations	L.M. Stevers (TU/e; Ottmann) Small-molecule stabilization of the binding between 14-3-3 and CFTR	S. Dharadhar (NKI; Sixma) A conserved two-step binding for the UAF1 regulator to USP12	D.W.H. Swenson (UvA; Vreede) Simulating the mechanisms and rates of transitions between Watson-Crick and Hoogsteen base pairing
12.05 - 12.25	P. Lössl (UU, Heck) Integrating MS-based approaches with cryo-EM defines the structural basis of cyanobacterial circadian timekeeping	M. Avalos (LEI; Van Wezel) Antimicrobial activity of volatile organic compounds (VOCs) produced by Streptomyces	I. Bernar (RU; Rutjes) Selective functionalization of aromatic heterocycles through hydroamination of alkoxyallenes	A.R. Blaazer (VU; De Esch) Biophysical interrogation of small-molecule binding to parasitic and human phosphodiesterases (PDEs)	M.C.E. van Dalen (UT; Post) A protein specific effect of amyloid micronetworks for cartilage tissue engineering	J. van den Berg (RUG; Poolman) Volume regulation and crowding homeostasis in Escherichia coli probed by super-resolution optical microscopy	B. Kleizen (UU; Braakman) Deciphering the mode of action of clinically relevant drugs developed against Cystic Fibrosis	A.S.Y. Wong (RU; Huck) Resilience in a family of enzymatic reaction networks	N. Hermans (LEI; Van Noort) Single Molecule Analysis of Chromatin Fragments of 18S rDNA from Yeast
12.25 - 13.55	Lunch & Poster session 'even' for PR, NA, LB, BMC, DS, SR, MC and AC posters (continued)								
Room	Room 55-57	Boszaal	Room 63/64	Room 58	Parkzaal	Auditorium	Room 82/83	Room 80/81	Room 65
	Imaging & Data handling Chair: Garry Cortals	Supramolecular Chemistry III Chair: Anja Palmans	Chemical Biology II Chair: Tom Wennekes	Bio-organic chemistry Chair: Thomas Boltje	Enzymology II Chair: Andy Thunnissen	Lipids in cell biology Chair: Dorus Gadella	Protein structure II Chair: Bert Janssen	Single molecule biophysics Chair: Menno Prins	Epigenetics Chair: Leonie Kamminga
13.55 - 14.15	Z. Ristanović (UU; Weckhuysen) Quantitative Real-time Chemical Imaging of Single Particle Reactivity in Dealuminated Zeolite ZSM-5 Crystals	R.P.M. Lafleur (TU/e; Meijer) Structural Diversity of a Supramolecular Polymer in Water as Revealed by H/D Exchange	M.E. Artola (LEI; Overkleef) Rational design of mechanism-based retaining glucosidase inhibitors	G.J.J. Richelle (UvA; Van Maarseveen) Scaffold-assisted peptide cyclizations: a new approach towards functional protein mimics?	I.K. Jóźwik (RUG; Thunnissen) Structural basis of steroid binding and selective oxidation by P450 monooxygenase CYP109E1	M. Giani (UT; Den Otter) Clathrin assembly regulated by adaptor proteins in coarse-grained models	D. Ugurlar (UU; Gros) Solving the mystery of C1: Structural insights into the first component of complement	C.P. Moerland (TU/e; Prins) Cardiac troponin conformation switching observed on the single molecule level by antibody-targeted nanomechanics	T. Korthout (NKI; Van Leeuwen) A maintenance mechanism for histone variant H2A.Z in dynamic promoter nucleosomes
14.15 - 14.35	J. Han (RUG; Horvatovich) Application of self-assembled Pd <sub>4</sub> L <sub>4</sub> metallocages in peptide/protein distribution imaging in tissue and drug delivery	K. Stout (RU; Elemans) Threading polymers through covalently linked double porphyrin cavities	J. Lohse (RUG; Witte) Diazotransfer reagents to selectively functionalize a protein of interest with azido groups	N. Tahiri (RUG; Minnaard) Chemical modifications of aminoglycoside antibiotics to combat bacterial resistance	T.A. Ewing (WUR; Van Berkel) Investigations into the mechanism and substrate specificity of vanillyl alcohol oxidase and eugenol oxidase	M.V. Baranov (RU; Van den Bogaart) Tethering of the peripheral actin cage to phagosomes	N.O.L. Leloup (UU; Janssen) The conformational changes that underlie the function of a sorting receptor	B. Pradhan (LEI; Canters) Fluorescence of fluorophores in lipid bilayers enhanced by gold nanorods	W.A.M. Hoeijmakers (RUMC; Bartfal) Reading the readers of the P. falciparum epigenome
14.35 - 14.55	A.M. Brunner (UU; Scheltema) Positional Isomer Monitoring by Top-down MS/MS	M. Kosian (WUR; Smulders) Structure and Long-Term Stability of Alkylphosphonic Acid Monolayers on Stainless Steel	F. Kleinpenning (RU; Bongor) Subcellular proteomic mapping by a spatially-restricted arylamine N-acetyltransferase	A. Pekosak (VU; Windhorst) Unprecedented Highly Stereoselective Radiosynthesis of Carbon-11 Labeled Small Peptides for PET Imaging	B. Srou (TUD; Hagedoorn) Pre-steady state kinetics of redox metalloenzymes	R.A. Korver (UvA; Testerink) Halotropism re-visited: biochemical fundamentals behind changes in root growth direction during salt stress	W.J. Keune (NKI; Perrakis) Steroid binding to Autotaxin links bile salts and lysophosphatidic acid signalling	D.M. van Elsland (LEI; Van Kasteren) Imaging bioorthogonal pathogens by correlative light-electron microscopy shows degradation of these pathogens in phagocytes	G. van Mierlo (RUMC; Marks) Dynamics of Polycomb localisation and abundance in pluripotency
14.55 - 15.15	G.H. Tinnevelt (RU; Jansen) Towards Single-Cell Omics With Novel Data Fusion Methods For Flow Cytometry	S. Mytnyk (TUD; Van Esch) Microstructured soft materials using aqueous multi-phase systems	D.T. Schmieden (TUD; Meyer) Using bacteria to make improved, nacre-inspired materials	I. Dijkgraaf (UM; Hackeng) Tetrameric NGR peptide as molecular imaging agent of neovascularization after myocardial infarction	F. Nami (LEI; Groenen) Rapid freeze-quench multi-frequency EPR: The enzymatic reduction of oxygen by small laccase	F. Campbell (LEI; Kros) Temporal Control of Membrane Fusion through Photolabile PEGylation of Liposome Membranes	F.Y. Ho (RUG; Kortholt) Biochemical and Structural analyses of the Parkinson's disease-related LRRK2 RocCOR domain.	T.L. Lenstra (NKI) Single-molecule imaging reveals switch between spurious and functional ncRNA transcription	B. Henneman (LEI; Dame) Dynamic and versatile DNA binding of archaeal histones
15.15 - 15.45	Snack Break								
15.45 - 16.15	Keynote: Thorsten Bach Technical University Munich (Room 63/64)  Chirality and Light: Enantioselective Catalysis of Photochemical Reactions			Keynote: Carsten Schultz European Molecular Biology Laboratory, Heidelberg (Room 82/83)  Tools for imaging and manipulating cellular networks			Keynote: David Leys University of Manchester (Auditorium)  Serendipitous discovery of enzymatic 1,3 dipolar cycloaddition: nature can put 2 and 3 together		
16.20 - 17.05	Plenary lecture: Georg Seelig University of Washington (Beneluxzaal)  Dynamic DNA nanotechnology from the test tube to the cell								
17.05 - 17.15	Announcement poster prizes day 2/3 and closure								

Analytical Chemistry

(Bio-)Organic chemistry

Medicinal Chemistry

Biochemistry & Molecular Biology

## Plenary speaker themed sessions and keynotes 6/7 December

10:10 – 10:55

Beneluxzaal

### **Plenary lecture: Clare Grey**

*Following Function in Real Time: Structure and Dynamics in Batteries and Supercapacitors*

The development of light, long-lasting rechargeable batteries has been an integral part of the portable electronics revolution. This revolution has transformed the way in which we communicate and transfer and access data globally. The invention of the lithium-ion (Li-ion) battery, a rechargeable battery in which lithium ions (Li<sup>+</sup>) shuttle between two materials (LiCoO<sub>2</sub> and graphitic carbon) has been an integral part of these advances. Rechargeable batteries are now poised to play an increasingly important role in transport and grid applications, but the introduction of these devices comes with different sets of challenges. Importantly, fundamental science is key to producing non-incremental advances and to develop new strategies for energy storage and conversion.

This talk will focus on our work on the development of methods that allow devices to be probed while they are operating (i.e., in-situ). This allows, for example, the transformations of the various cell components to be followed under realistic conditions without having to disassemble and take apart the cell. To this end, the application of new in and ex-situ Nuclear Magnetic Resonance (NMR), magnetic resonance imaging (MRI) and X-ray diffraction approaches to correlate structure and dynamics with function in lithium-ion and lithium air batteries and supercapacitors will be described. The in-situ approach allows processes to be captured, which are very difficult to detect directly by ex-situ methods. For example, we can detect side reactions involving the electrolyte and the electrode materials, sorption processes at the electrolyte-electrode interface, and processes that occur during extremely fast charging and discharging. Complementary Ex-situ NMR investigations allow more detailed structural studies to be performed, to correlate local and long-range structure with performance.

After a general overview of our in situ NMR and MRI studies on batteries and supercapacitors, this talk will focus on our recent work on olivines, spinels and Ge/Si anodes. The development of new NMR approaches to investigate paramagnetic battery materials, both in and ex situ, will be discussed, the approach making use of both theory and experiment. Although it is difficult to achieve high-resolution spectra from these paramagnetic materials in the in situ experiments, measurements of the relaxation time allow access to the dynamics of the lithium ions in real time as a function of state of charge. Finally, the use of NMR spectroscopy, in the study of disordered and amorphous anode materials will be described.

## Plenary speaker themed sessions and keynotes 6/7 December

### THEMED SESSION: X-ray experiments of Materials and Catalysis

Chair: Frank de Groot

Boszaal

14:00 – 14:30

#### Florian Meirer (UU)

*X-ray microscopy at multiple length scales – the showcase of metal poisoning of catalyst particles*

F. Meirer

Inorganic Chemistry and Catalysis, Utrecht University, 3584 CG Utrecht, The Netherlands

Modern X-ray imaging techniques allow for the combination of high spatial resolution, a large field of view, short dwell times, and the capability to obtain spectroscopic information. This has opened the door to high-resolution studies correlating chemistry and morphology of, for example, whole catalyst particles used in fluid catalytic cracking (FCC).

FCC is an important process in petrochemical industry, accounting for 40-45% of worldwide gasoline production. In FCC, catalyst particles are employed to crack large hydrocarbon fractions into more valuable materials, such as gasoline and propylene [1]. During operation the catalyst accumulates poisonous metals that have been related to catalyst deactivation. However, detailed knowledge about metal deposition mechanisms as well as the deposition's effects on particle morphology and chemistry is limited.

In this presentation I will summarize our recent studies of individual FCC catalyst particles using synchrotron based hard X-ray full field transmission X-ray microscopy [2,3,4,5], hard X-ray fluorescence tomography [5,6], and soft X-ray ptychographic imaging [7], highlighting the possibilities offered by modern X-ray microscopy.

#### References

[1] E.T.C. Vogt, B.M. Weckhuysen, Chem. Soc. Rev. 44, 7342-7370 (2015).

[2] F. Meirer, D.T. Morris, S. Kalirai, Y. Liu, J.C. Andrews, B.M. Weckhuysen, J. Am. Chem. Soc. 137, 102–105 (2015).

[3] F. Meirer, S. Kalirai, J. Nelson Weker, Y. Liu, J.C. Andrews, B.M. Weckhuysen, Chem. Commun. 51, 8097–8100 (2015).

[4] F. Meirer, S. Kalirai, D. Morris, S. Soparawalla, Y. Liu, G. Mesu, J. C. Andrews, B. M. Weckhuysen, Science Advances 1, e1400199 (2015).

[5] Y. Liu, F. Meirer, C.M. Krest, S. Webb, B.M. Weckhuysen, Nature Communications 7, 12634 (2016).

[6] S. Kalirai, U. Boesenberg, G. Falkenberg, F. Meirer, B.M. Weckhuysen, ChemCatChem 7, 3674-3682 (2015).

[7] A.M. Wise, J. Nelson Weker, S. Kalirai, M. Farmand, D.A. Shapiro, F. Meirer, B.M. Weckhuysen, ACS Catal. 6, 2178–2181 (2016).

14:30 – 14:50

#### Moniek Tromp (UvA)

*The active site in the spotlight!*

Detailed information on the structural and electronic properties of a catalyst or material and how they change during reaction is required to understand their reaction mechanism and performance. High energy x-rays expose the detailed electronic properties and structure providing information on the oxidation states, type of atoms, their position and geometry. This so-called x-ray absorption spectroscopy (XAS) can be applied while the catalysts are working, providing structure-performance and mechanistic insights.

XAS has mostly been used to obtain a structural picture whereas the electronic structure is often poorly understood. Moreover, XAS is a macroscopic technique, providing an average of all the different species present. New developments, in which specific x-ray energies are selected, provide more detailed electronic information and can make the technique more specific. Other developments focus on the increase of time resolution, allowing one to follow reactions down to the sub-millisecond to pico-second time regime, and characterizing different parts of the molecules.

These X-ray techniques are currently being developed and applied to catalytic systems and materials. In this lecture I will show you some of the concepts behind the X-ray techniques, and demonstrate their strengths in important (industrial) processes (e.g. catalysis and batteries).



## Plenary speaker themed sessions and keynotes 6/7 December

14:50 – 15:10

**Jan-Philip Hoffman (TU/e)**

*Synchrotron-based X-ray Structural Analysis of Functional Materials Towards Catalytic Structure-Performance Relationships*

Laboratory of Inorganic Materials Chemistry, Department of Chemical Engineering and Chemistry, Eindhoven University of Technology, P.O. Box 513, 5600MB Eindhoven, The Netherlands  
j.p.hofmann@tue.nl

Heterogeneous catalysis plays a significant role in chemical industry. To arrive at a knowledge-based catalyst design, fundamental insight into relations between structure and catalytic properties, such as activity, selectivity and stability, is needed. During this lecture, examples from recent synchrotron-based work performed at ESRF will be highlighted. Showcase examples will include augmented micro-XRD on model zeolites, operando surface X-ray diffraction and reflectivity under electrochemical conditions as well as in-situ coherent X-ray diffraction imaging of individual catalyst nanoparticles under conditions of gas-phase and electrocatalysis.

## Plenary speaker themed sessions and keynotes 6/7 December

### THEMED SESSION: Chemistry at the nanoscale

Chair: Joost Reek

Auditorium

14:00 – 14:30

**Wesley Browne (RUG)**

14:30 – 14:50

**S. Gonell (UvA, Reek)**

*Catalysis at extremely high local concentrations by catalyst confinement in M12L24 nano-cages*

Catalysis is usually carried out using catalyst concentrations in the micro-milimolar range. We have developed supramolecular strategies to pre-organise metal complexes in confined space leading to local concentrations in the molar range. This high concentration leads to increased reactivity for a variety of reactions which will be discussed in this contribution

14:50 – 15:10

**S. Wezenberg (RUG)**

*Allosteric regulation of the rotational speed in light-driven molecular motors*

Synthetic molecular rotary motors, in particular those that are driven by light, are highly promising for controlling the motion of nanoscale systems. To reach the same level of sophistication and complexity as is found in biological motors, however, it is crucial to design strategies that allow for dynamic modulation of the rotational behavior. To address this challenge, we have developed an overcrowded alkene-based motor that binds to metal ions. The rotational speed of this motor can be tuned via the reversible complexation with different transition metals, which represents a significant step toward integrated chemical regulation in light-operated nanomechanical devices.

## Plenary speaker themed sessions and keynotes 6/7 December

### THEMED SESSION: Process Intensification and Flow Chemistry - 1

Chair: Andrzej Stankiewicz

Room 58

14:00 – 14:30

#### **M. van Sint-Annaland (TU/e)**

*Fluidised bed membrane reactors for ultra-pure H<sub>2</sub> production*

Based on process intensification by process integration, novel energy and carbon efficient process concepts for hydrogen production with integrated CO<sub>2</sub> capture are being developed, exploiting the synergetic effects when combining reaction and separation in a single multifunctional reactor. In particular for the production of ultra-pure hydrogen, the integration of hydrogen perm-selective membranes in fluidized-bed reactors has shown great potential, particularly for small-scale distributed production. In this presentation the current state-of-the-art of fluidized bed membrane reactors for H<sub>2</sub> production is being reviewed, and the ongoing developments will be shown and discussed concerning: i) the preparation of supported ultra-thin Pd/Ag membranes (long-term stability and permselectivity, H<sub>2</sub>S resistance); ii) catalyst development for integration in membrane reactors; iii) lab-scale reactor demonstration and iv) quantification of mass transfer processes and concentration polarization effects, investigated by advanced non-invasive optical techniques and numerical modelling; v) comparison with other novel reactor concepts such as chemical looping reforming.

14:30 – 14:50

#### **M. Escriba-Gelonch (TU/e, Hessel)**

*Continuous processing of Vitamin D<sub>3</sub> with integrated high-T photo flow chemistry and antisolvent crystallization*

An integrated synthesis-crystallization micro-flow system is presented for the continuous production of crystalline Vitamin D<sub>3</sub>. The aim is to intensify the handling of the product in the following formulation process steps. A novel photo-high-T microflow vitamin D<sub>3</sub> synthesis set-up is directly coupled to a continuous antisolvent crystallization process. Here, solvents are swapped in-flow in order to enhance the supersaturation. Microfluidic measures will assist intense particle nucleation, leading to many small initial crystals, and is followed by crystal growth in a subsequent cool step. XRD confirms that the white crystals obtained present the most stable polymorphism according to the art.

14:50 – 15:10

#### **M.A. Reus (TUD, Stankiewicz)**

*Crystallization in composite hydrogels for controlling polymorphism*

This study aims to control the polymorphism in model API nanocrystals through interplay of confinement and interactions between surfactant molecules at liquid-liquid interfaces. We immobilize so called nanoemulsions of solution in a hydrogel matrix and crystallize the API through evaporation. For the crystallization of griseofulvin (GRIS) from the solvent anisole (ANI), the resulting product had a different XRPD pattern than GRIS crystallized from ANI in 1 mL solution volumes. The same was observed for the solvent dichloromethane (DCM). This difference indicates that the polymorph crystallized inside the small emulsion droplets was not the same as that crystallized in the bulk and that the crystallization in the composite hydrogel can control the polymorphism.

## Plenary speaker themed sessions and keynotes 6/7 December

### THEMED SESSION: Molecular Assemblies

Chair: Albert Schenning

Parkzaal

14:00 – 14:30

#### Tom de Greef (TU/e)

*System-level investigations of one-dimensional self-assembly*

Organic supramolecular polymers including pi-conjugated nanowires, nanotubes etc. represent a novel class of materials for miniaturized devices as their properties have unique characteristics different than the bulk material. While several thermodynamic self-assembly mechanisms of these one-dimensional nanomaterials in solution have been identified, the effect of competing, kinetically-controlled self-assembly pathways, the role of co-solvents in the formation of these structures and seed-induced growth are poorly understood. Therefore, in order to advance the field, it is critical that these effects are studied and generalized at the system level which requires a combination of carefully designed experiments and theoretical modeling.

Using kinetic nucleation-elongation theories originally developed to describe the formation of amyloid protein-based fibers, I will show how these models can be extended to incorporate the effect of kinetically controlled pathways as well as the effect of denaturants (i.e. good solvents) and pre-formed seeds on self-assembly kinetics. Several counterintuitive effects such as a slowing down of self-assembly kinetics at high concentrations or intermediate denaturant concentrations will be explained in a quantitative manner. Importantly, the simulations will be guided by kinetic experiments. This detailed kinetic characterization sets the stage towards the formulation of a general set of design rules which will make a model-driven, programmable approach towards molecular self-assembly of one-dimensional nanomaterials possible. Such efforts will aid in the development of organic photovoltaic devices, dynamic biomaterials and chemical sensors.

14:30 – 14:50

#### N. Tiwari (Tue, van der Schoot)

*Mixing kinetics of reversible copolymerization*

The equilibrium and kinetic properties of the irreversible self-assembly of two types of monomers also known as the copolymerization, has been studied extensively in the literature. However, little attention has been given to reversible copolymerization mainly due to the additional conformational information that is needed to completely describe such systems. In this work, we study the reversible step growth copolymerization with the terminal effect, where only the end monomer dictates the rate of monomer addition or removal. To properly account for reversibility, we derive the conditional probabilities for the terminal pair, assuming the local conformational equilibrium. Solving the resulting hierarchy of rate equations numerically we investigate the mixing kinetics of the copolymers, i.e., the evolution of the conformation of the copolymers as a function of time. We focus on how the mixing kinetics depends on the concentration of monomers as well as on affinity between the two types of co-monomer. We find that the time scale of mixing follows a power law in concentration and the affinity between the two co-monomers.

14:50 – 15:10

#### I. Kryven (UvA, Bolhuis)

*Multilayer approach to modelling of interconnected soft matter structures*

Assembly of molecular networks from multifunctional precursors, that are dynamically evolving themselves (e.g. as in polymerisation of Triglycerides or tetra-functional PEG hydrogels) is a typical process requiring the multilayer coarse-graining. We consider a hybrid model that incorporates the reaction kinetics for precursors and a random graph process explaining evolution of the network topology. The process does not account for spatial positions of the monomers explicitly, yet the Euclidean distances between the monomers are derived from the topology. The model is compatible with large space/time scales, and thus allows one to study gels qua a single molecule.

## Plenary speaker themed sessions and keynotes 6/7 December

### THEMED SESSION: Disentangling chirality with spectroscopy

Chair: Wybren Jan Buma

Room 63/64

14:00 – 14:30

#### **Maurice Janssen (MassSpecpecD)**

*Direct enantiomer selective Mass Spectrometry of chiral molecules by MS-PECD*

Mass Spectrometry is chirally blind, it cannot directly distinguish the two enantiomers of chiral molecules. Simultaneous, enantiomer-specific identification of chiral molecules in multi-component mixtures is extremely challenging. Here we show how enantiomers may be differentiated by Mass-Selected PhotoElectron Circular Dichroism (MS-PECD) using an electron-ion coincidence imaging spectrometer [1]. Following an ionizing circular polarized laser pulse, ions and electrons are detected in coincidence on their respective time- and position sensitive detectors. The Mass-Selected PECD reveals that the compound is chiral.

[1] M.H.M. Janssen & I. Powis, PCCP, 16, 856 (2014); M. M. Rafiee Fanood et al., Nature Communications 6, 7511 (2015)

14:30 – 14:50

#### **P. Nicu (Uva, W.J. Buma)**

*The generalized coupled oscillator VCD mechanism and its implications for the interpretation of VCD spectra*

A critical analysis of the coupled oscillator (CO) model for VCD is performed by casting the rotational strength (R) into a form that contains explicitly the coupled-oscillator expression. This theoretical analysis has led to the introduction of a generalized coupled oscillator (GCO) mechanism that is intrinsically exact and has a much more general character. As will be shown using a few illustrative examples, this mechanism acts as a general VCD enhancement mechanism and affects the intensities of all types of normal modes (i.e., not just C=O stretching modes) in both symmetric and asymmetric molecules.

14:50 – 15:10

#### **Huib Bakker (Amolf)**

*Probing the absolute configuration of chiral molecules at aqueous interfaces*

We demonstrate that enantiomers of chiral macromolecules at the surface of water can be distinguished with monolayer sensitivity using heterodyne-detected vibrational sum-frequency generation (VSFG) spectroscopy. We use a polarization combination that selectively probes chiral molecular structures, and we determine the phase of the sum-frequency light produced by the chiral molecules by interfering this light with the light of a local oscillator. The phase of the VSFG light directly reflects the handedness of the probed chiral molecules. We use the technique to distinguish left-handed and right-handed helical isomers of anti-freeze protein type I peptides at the surface of liquid water.



## Plenary speaker themed sessions and keynotes 6/7 December

### KEYNOTES

Wednesday 7 december 2016  
08.30 – 09.00

Room 82/83

**Wybren Jan Buma (UvA)**

*High-resolution laser spectroscopy of photoactive materials: light on the dark side of the force*

Absorption of light brings molecules into an activated state. From this state radiative processes can occur, but what is much more interesting are the nonradiative, dark processes in which the energy of the photon is transformed into other forms of energy such as mechanical and chemical energy. It are these light-to-activity pathways that we want to learn to control as they ultimately allow us to use photon energy to drive targeted applications such as energy conversion, photocatalysis, photon-driven molecular nanotechnology, as well as optogenetics and photopharmacology.

Key to tailoring photoactivity are studies of potential energy surfaces of electronically excited states that are accessed, preferably first under isolated conditions. Such studies provide insight on changes in the electronic structure of the molecule upon excitation and the forces that act on the molecular structure. They map out which coordinates are involved in the structural dynamics, reveal whether energy barriers are involved, and provide a direct benchmark for theoretical calculations. They are also, however, a necessary starting point for a further appreciation -and rational use- of the dependence of photodynamical phenomena on environment and substituents.

Photoactivity is generally associated with (ultra)fast conversions of energy. It has therefore for a long time been taken as an unspoken rule that the application of 'slow' spectroscopies such as high-resolution nanosecond laser spectroscopies to study photoactivity is intrinsically a contradiction in terms. Using eye-catchers from molecular nanotechnology, health care, and various areas where photochromic compounds are employed, we have shown in recent years that quite the opposite is true. This is exciting as there is a huge amount of photoresponsive systems that so far have been discarded for such studies because their lifetimes were considered to be prohibitively short. There is thus still much to be learnt on the dark side of the forces that act upon molecules after light absorption.

Auditorium

**IJla Voets (Eindhoven Univ. of Technology)**

*Hot proteins on cool crystals: crystal growth modulation by ice-binding proteins*

Crystallization of water into ice is lethal to most organisms and detrimental to many soft materials. Freeze-avoiding fish living in polar seas have evolved to tackle this problem with an unusual coping strategy. They produce so-called antifreeze proteins (AFPs) that block the growth of nascent ice crystals within a narrow temperature range known as the thermal hysteresis gap enabling survival under extreme conditions [1]. Encoding this functionality into synthetic polymers would open up new avenues for e.g. cryopreservation, de-icing technologies and advanced coatings.

We study how and why ice-binding proteins (IBPs) bind onto specific ice crystal planes and its impact on the various functional roles of ice-binding proteins (freezing point depression, inhibition of recrystallization, crystal shaping, etc.) using a range of activity assays [1, 2]. We aim to achieve a solid mechanistic understanding of how IBPs work as a crucial first step for the knowledge-based design of potent synthetic ice crystal growth modifiers.

An evaluation of thermal hysteresis (TH) and ice recrystallization inhibition (IRI) activity of all major classes of AFPs using cryoscopy, sonocrystallization, and recrystallization assays reveals a marked difference in TH activities determined by cryoscopy and sonocrystallization, while TH and IRI activities are not correlated [2]. This points to a mechanistic difference in ice growth inhibition by various types of AFPs: basal plane adsorption is relevant only at long annealing times and at small undercooling, while blocking fast ice growth requires rapid adsorptions on other crystal planes. Interestingly, an ice-like vibrational signature is observed in the sum frequency generation (SFG) spectrum taken at room temperature of the only antifreeze protein that displays virtually the same TH activity (Figure 1) in cryoscopy (slow growth) and sonocrystallization (fast growth), suggesting that ice-binding of this protein (rQAE) is mediated by its hydration shell [3]. The characteristic ice-like feature disappears upon a single point mutation in the ice-binding site from threonine to asparagine, which also eliminates activity. These findings shed light on the working mechanism of IBPs and offer direction to design synthetic macromolecular antifreezes [4].

## Plenary speaker themed sessions and keynotes 6/7 December

Room 63/64

**Joost Reek (Univ. of Amsterdam)**

*Catalysis in self-assembled confined spaces: Control of catalyst properties by the second coordination sphere*

The interface between supramolecular chemistry and transition metal catalysis has received surprisingly little attention in contrast to the individual disciplines. It provides, however, novel and elegant strategies that lead to new tools for the search of effective catalysts, and as such this has been an important research theme in our laboratories. In this presentation I will focus on supramolecular strategies to control activity and selectivity in transition metal catalysis, which is especially important for reactions that are impossible to control using traditional catalyst development. For substrates with functional groups we use substrate orientation effects to control selectivity, whereas for non-functionalized substrates we create cages around the active transition metal. In addition, the application of a cofactor strategy will be presented, which is also ideally suited for combinatorial approaches. What these strategies have in common is the contribution of the second coordination sphere to the catalytic properties, which is quite different from the traditional ligand effects.

## Abstracts parallel lectures 6/7 December

### Room 55/57 Photocatalysis and Solar Fuels

6<sup>th</sup> December 2016, 11:15 – 11:35

*Site-Selectively Patterned NiMo on Silicon Micropillars with Radial pn-Junction for Unprecedented Hydrogen Production*

Wouter Vijselaar (UT), Janneke Veerbeek, Roald M. Tiggelaar, Han Gardeniers, Jurriaan Huskens

Solar fuels are the next generation in energy storage. Hydrogen out of water and sunlight is one of the possible candidates. The way to obtain high efficiencies for hydrogen production, is by decoupling the optical absorption and catalytic activity of the electrocatalyst. This allows for simultaneous achieving of high fill factors, photo-current density and open circuit values, and thus high efficiencies. We investigated how to achieve the above described statement with silicon as light absorber and Ni-Mo as co-catalyst, by fabricating Si micropillar PV cells with radial junctions and patterning these micropillars with high mass-loadings of catalyst.

6<sup>th</sup> December 2016, 11:35 – 11:55

*In operando characterization of light-induced charge variations of photocatalytically active TiO<sub>2</sub> surface by AFM*

Igor Siretanu (UT), Damon Rafieian, Guido Mul, Rob Lammertink, Frieder Mugele

We use AFM spectroscopy to quantify in situ the light-induced variation of the surface charge  $\sigma$  of sputter-deposited TiO<sub>2</sub> films immersed in an aqueous electrolyte solution.  $\sigma$  is found to decrease from approx. 0.1 e/nm<sup>2</sup> (at pH6 in dark) to almost zero upon UV illumination for films deposited on p-Si substrates. No response is found on n-Si. This AFM response coincides with a 100 times enhanced photocatalytic activity on p-Si vs. n-Si in dye degradation experiments in a microreactor device. Our results suggest an electron transfer-based mechanism of the photocatalytic reaction, presumably involving dissolved O<sub>2</sub>.

6<sup>th</sup> December 2016, 11:55 – 12:15

*Charge Carrier Behaviour in MOFs developed for Photocatalytic Applications*

J.H.J. Wijten (UU),

In the past few years the potential of metal-organic frameworks (MOFs) for photo-catalytic applications has been explored. MOFs are often regarded as versatile materials as their constituting building blocks, namely metal centres and organic linkers, can be varied, leading to a wide variety of properties. However, little is understood how the composition and connection of these building blocks affect the physicochemical properties. In this research we aim to shed some light on the relation between the metal centres and organic linkers with their optical properties. With these results we hope we can further the development of MOFs for photo-catalytic applications.

## Abstracts parallel lectures 6/7 December

### Boszaal: Cooperative ligand design

6<sup>th</sup> December 2016, 11:15 – 11:35

#### *Synthesis and Reactivity of Nickel Complexes Bearing a Non-Innocent Diphosphine Ketone ligand*

Alessio F. Orsino (UU), Dide G. A. Verhoeven, Bartholomeus W. H. Saes, Martin Lutz, Robertus J. M. Klein Gebbink, Marc-Etienne Moret

The replacement of precious metals by base metal systems has gained significant attention in the field of catalysis, as it pairs with sustainable chemistry. This research targets the development of nickel-based catalysts, incorporating a diphosphine ketone ligand, where the C=O moiety can be bound in  $\eta^2$ -coordination mode. In this presentation, the hemilabile and the acceptor character of the ligand is described. The hemilability of the C=O bond was observed during the catalytic cyclotrimerisation of alkynes. In addition, the cooperative behaviour of the ligand was demonstrated by the reaction with methyl triflate, turning the ketone moiety into an alkoxyalkyl group.

6<sup>th</sup> December 2016, 11:35 – 11:55

#### *Synthetic Applications of Cobalt(III)-Carbene Radicals*

Colet te Grotenhuis (UvA), Braja Gopal Das, Bas de Bruin

In this contribution we will discuss the reactivity of cobalt(II) towards carbene precursors, leading to formation of cobalt(III)-bound substrate radicals. These "carbene radicals" are key-intermediates in a series of interesting catalytic transformations involving ring-closure and double-bond formation useful in organic synthesis.

6<sup>th</sup> December 2016, 11:55 – 12:15

#### *Versatile Reactivity and Catalysis of Lutidine-based Ligands with Transition Metal and Main Group Elements*

Marc Devillard (UvA), Jarl Ivar van der Vlugt

The use of proton-responsive (phosphinomethyl)pyridine ligands in transition-metal catalysis is known to facilitate the activation of E-H bonds at the TM center.

We developed silyl-decorated ligands of this type that give access to unprecedented bimetallic TM complexes featuring reactive metal-C bonds. The peculiar bonding situation within these complexes allows for versatile reactivity toward E-H bonds.

On the other hand, we have extended the coordination chemistry of pyridine-based ligands to p-block Lewis acids in order to replace TM by abundant and cheap elements. The stability and reactivity of intramolecularly stabilized silylium ions in small molecule activation will be discussed.

## Abstracts parallel lectures 6/7 December

### Room 58: Catalytic and Nano Engineering

6<sup>th</sup> December 2016, 11:15 – 11: 35

*Controlled Growth of Metal Nanoparticles on Substrates via Scalable Atmospheric Pressure Atomic Layer Deposition*

Fabio Grillo (TUD), Hao Van Bui, Michiel T. Kreuzter, J. Ruud van Ommen

We demonstrate the deposition of crystalline metal nanoparticles on substrates such as graphene via atmospheric pressure atomic layer deposition (ALD). We carry this out in a reactor in which the substrate is dispersed in the gas phase, enabling the production of large amount of material. By analysing the evolution of the particle size distribution and spatial density, we obtained insights into the nucleation and growth of metal ALD. Such insights enable us to tailor the particle size distribution and loading of the noble metal clusters.

6<sup>th</sup> December 2016, 11:35 – 11: 55

*On the adsorption of CO<sub>2</sub> and H<sub>2</sub>O on hydrotalcite-based sorbents*

Kai Coenen (TU/e), Fausto Gallucci, Paul Cobden, Hemiel Hensen, Martin van Sint Annaland

The adsorption behavior of carbon dioxide and water on a K-promoted hydrotalcite based adsorbent has been studied by thermogravimetric analysis and packed bed reactors to elucidate the effect of steam addition to the sorption capacity of hydrotalcite sorbents for WGS reaction.

6<sup>th</sup> December 2016, 11:55 – 12:15

*Synthesis and deposition of non-toxic, stable colloidal semiconductor nanocrystals for lighting and photovoltaic applications*

Ryan W. Crisp (TUD), Laurens D.A. Siebbeles, J. Ruud van Ommen, Arjan J. Houtepen

Colloidal semiconductor nanocrystals (NCs) are promising for lighting and photovoltaic applications because (among other reasons) their spectral response is highly dependent on the NC size – a readily tuneable parameter. Past research focused on materials that contain lead or cadmium, thus not generally suitable for commercialization. To move beyond non-toxic Pb- and Cd-containing NCs requires development of new synthetic procedures controlling both the NC size but also engineering the composition to improve the optoelectronic properties like photoluminescence quantum yield and charge transport. Here, we present work on developing indium-based NCs to meet the many challenges involved in LEDs and solar cells.



## Abstracts parallel lectures 6/7 December

### Parkzaal: Microscopy of Soft matter

6<sup>th</sup> December 2016, 11:15 – 11:35

*Imaging the topology of soft and deformable interfaces by single-molecule localization microscopy*  
Antonio Aloï (TU/e), Neus Vilanova, Lorenzo Albertazzi, Ilja K. Voets

Soft and deformable interfaces are difficult to image in-situ, in a non-invasive manner with nanometric resolution. To tackle this challenge we developed a single molecule localization microscopy (SMLM) technique capable of resolving the topology of objects without the need for covalent labelling: interface Point Accumulation for Imaging in Nanoscale Topography (iPAINT) [1]. iPAINT is based on the reversible, aspecific physisorption onto interfaces of polymer chains end-functionalized with a photo-activatable moiety. We demonstrate herein its potential for visualization of air nanobubbles, measurements of the contact angles of single colloidal particles at fluid interfaces, and monitoring morphological anisotropies of complex core-shell micelles.

References:

1. A. Aloï, N. Vilanova, L. Albertazzi, I. Voets, *Nanoscale*, 2016, 8, 8712-8716.

6<sup>th</sup> December 2016, 11:35 – 11:55

*Quantitative Multiscale Electron Microscopy of Functional Materials*  
Heiner Friedrich (TU/e),

To enable progress in synthesis and assembly of novel functional materials, electron microscopy (EM) is a key tool. Beyond conventional EM, where one has to choose between either high resolution images or large fields of view at low resolution, quantitative multiscale EM is now emerging. This approach facilitates the study of materials properties that arise from interactions between individual components over multiple length scales. On examples of conductive colloids, the relationships between size, processing, final packing and electrical conductivity are detailed. Particular emphasis is placed on the role of quantification to ensure that representative sample volumes are probed.

6<sup>th</sup> December 2016, 11:55 – 12:15

*Angle-dependent single chain adhesion of polymers by AFM*  
Lucie Grebikova (UT), Bart D. Kieviet, G. Julius Vancso

We have introduced direction control into single polymer adhesion force measurements, in order to describe how the polymer adsorption-desorption behavior depends on the angle at which the force is applied. The adhesion of poly(2-hydroxyethyl methacrylate) (pHEMA) end-grafted to the atomic force microscopy tip was studied on a planar surface in solution by single molecule force spectroscopy. Our experiments indicate that the magnitude of desorption force changes with the pulling angle and there is a critical angle beyond which the polymer cannot be desorbed by applying a force.

## Abstracts parallel lectures 6/7 December

### Auditorium: Responsive Supramolecular Systems

6<sup>th</sup> December 2016, 11:15 – 11:35

*Large amplitude light-driven motions in liquid crystal networks*  
Anne Hélène Gelebart (TU/e),

Liquid crystal networks (LCN) can be implemented with a photoresponsive molecule in order to achieve large macroscopic deformation. Those photoresponsive LCN represent a nice playground and many applications can be achieved using their anisotropic properties and alignment versatility. An easy and potentially scalable method to produce an array of photoresponsive fibers has been developed. All the fibers are able to largely and reversibly bend at room temperature in a cooperative manner. Furthermore, when immersed in a liquid, the fibers create a directional flow leading to transportation of floating objects in a desired direction.

6<sup>th</sup> December 2016, 11:35 – 11:55

*Supramolecular polymers from a different angle – The characteristics and limits of single-chain folding*  
Gijs M. ter Huurne (TU/e), Lafayette de Windt, Ilja K. Voets, Anja R. A. Palmans, E.W. Meijer

By combining the fields of small molecule self-assembly and polymer chemistry, unique macromolecular architectures can be obtained. Such single-chain polymeric nanoparticles (SCPNS) are highly interesting because of their resemblance to proteins, as well as their unique ability to create nanoparticles with well-organized structured domains that are suited for catalysis, sensing and drug delivery applications. Since structure and function are closely related, we aim to acquire more in-depth insight in the folding behavior, structure and the dynamics of such systems. Hereto, we study polymers grafted with structuring supramolecular motives using the combination of various spectroscopic and scattering techniques.

6<sup>th</sup> December 2016, 11:55 – 12:15

*Chemistry-Driven Supramolecular Architectures*  
Björn Kriete (RUG),

Supramolecular structures of amphiphilic dye molecules such as micelles, bilayer sheets, single- or multiwall tubes have excelled as promising candidates for artificial light harvesting complexes as they comprise the peculiar excitonic transport properties with self-assembly capabilities. Gaining control over the assembly process requires fine tuning at the molecular level, but ultimately allows for making deliberate modifications to the optical properties without affecting the ability to self-assemble. Here we show how minimalistic changes to the chemical structure of the initial molecule lead to the formation of aggregates with significantly different molecular architectures.

## Abstracts parallel lectures 6/7 December

### Room 82/83: Solar energy conversion

6<sup>th</sup> December 2016, 11:15 – 11:35

#### *New approach in constructing highly efficient near infrared light upconversion nanomaterials*

Jing Zuo (UvA), Langping Tu, Yansong Feng, Xiaomin Liu, Xianggui Kong, Hong Zhang

Effective upconversion of continuous wave near infrared light to UV/Visible light in nanomaterials has significant potential in broad applications, e.g. photocatalysis, solar energy utilization, optical imaging and traceable drug carrier. These potentials are, however, dimmed by the unsatisfied efficiency of the most promising lanthanide doped complexes. Current approaches are failed to make further improvement. Our new nanostructure, based on the analysis of excitation energy migration dynamics in the confined systems, has led to unprecedented high monochromatic upconverted emission, which may lead to a new route in lifting upconversion efficiency. Proof of concept of applications will be provided in this presentation.

6<sup>th</sup> December 2016, 11:35 – 11:55

#### *Solid-state NMR study of perovskite bulk and thin films for solar cell applications*

Wouter M.J. Franssen (RU), Riza Dervisoglu, Bardo J. Bruijnaers\*, René A.J. Janssen\*, Arno. P.M. Kentgens

In recent years hybrid organic-inorganic halide perovskites have become the focus of attention because of the astonishing performance in photovoltaic applications. It is clear that the development of high efficiency solar cells based on these materials has outpaced the underlying understanding of the physical chemistry that is involved. We use multinuclear solid state NMR to study the structure and dynamics of both the organic and inorganic moieties in bulk methyl-ammonium lead halides. Subsequently the effects of processing are investigated, in order to get insight in factors affecting morphology, composition and stability, resulting in efficient thin film solar cells.

6<sup>th</sup> December 2016, 11:55 – 12:15

#### *Cu<sub>2</sub>O and CuS Nanoparticles: Preparation and Photocatalytic Performance*

Gang Wang (UU), Roy van den Berg, Koen W. Bossers, Ellen G. Heuven, Krijn P. de Jong, Celso de Mello Donega, Petra E. de Jongh

Cu<sub>2</sub>O and CuS are p-type semiconductors which attract much attention for application in photocatalysis. We explored new strategies to assemble these Cu-based semiconductor nanoparticles with controlled size and tunable optical properties using mesoporous silica supports. The activity, stability and selectivity of the as-obtained Cu<sub>2</sub>O and CuS nanoparticles, for different sizes, were examined for solar-driven H<sub>2</sub> evolution and in photocatalytic oxidation. A few examples will be highlighted, such as the size effect of silica-supported Cu<sub>2</sub>O nanoparticles on activity, and the possibility to influence the selectivity of the photocatalyzed oxidation reactions with CuS nanoparticles.

## Abstracts parallel lectures 6/7 December

### Room 63/64: Theory development

6<sup>th</sup> December 2016, 11:15 – 11:35

#### *Quantum Monte Carlo for transition metal containing dimers*

Katharina Doblhoff-Dier (LEI), Jörg Meyer, Philip E. Hoggan, Lucas K. Wagner, Geert-Jan Kroes

Transition metals (TMs) are omnipresent in many physically interesting systems, such as heterogeneous catalysts. However, they are notoriously difficult to describe theoretically. Diffusion Monte Carlo (DMC) offers the possibility to incorporate electronic correlation explicitly while still being scalable to large or periodic systems. We investigated a database of binding energies of TM containing dimers using DMC, which allows us to compare to accurate experimental results and other quantum chemical methods. Our results constitute essential guidelines for the assessment of achievable accuracy and the design of future QMC calculations on complex systems containing TM atoms.

6<sup>th</sup> December 11:35 – 11:55

#### *Local multi-resonance description of electronic excited states in quantum Monte Carlo*

Habiburrahman Zulfikri (UT), Claudia Filippi

The accurate, yet affordable, computation of excited states in large molecules remains a challenge in computational chemistry. Using the familiar concepts of local orbitals and Lewis resonance structures, we introduce here a new class of accurate many-body wave functions specifically designed for the efficient treatment of excited states in quantum Monte Carlo. We elaborate a coupling scheme between electrons within domains of local orbitals and combine it with the use of multiple Lewis structures. We demonstrate the good performance of our wave functions on prototypical retinal models and present preliminary results for their application to large chromophores of photosensitive proteins.

6<sup>th</sup> December 2016, 11:55 – 12:15

#### *Nonorthogonal configuration interaction for calculating the singlet fission efficiency*

Meilani K. Wibowo (RUG), Ria Broer, Remco W.A. Havenith

The elucidation of the mechanism of singlet fission is important for the development of new materials for organic photovoltaics. From calculations it can be deduced which parameters determine the singlet fission efficiency, and which states are involved in the transition from the photoexcited state to the singlet coupled triplet states. The rates of these radiationless processes are governed by the electronic coupling between these states. We have developed a nonorthogonal configuration interaction method for the calculation of this electronic coupling, which enables an interpretation in molecular excited states. The method will be explained and applied to potential singlet fission molecules.

## Abstracts parallel lectures 6/7 December

### Room 65: Dynamics and reactions

6<sup>th</sup> December 2016, 11:15 – 11:35

#### *Unraveling Molecular Collisions*

Jolijn Onvlee, Sjoerd N. Vogels, Gerrit C. Groenenboom, Ad van der Avoird, and Sebastiaan Y.T. van de Meerakker

Molecular collisions play an important role in the interstellar medium, atmospheres, and combustion. We combine high-resolution collision experiments with state-of-the-art scattering calculations to get detailed insights into molecular collision dynamics. Experimentally, we were able to observe diffraction oscillations and scattering resonances, for instance. These structures are a testimony of the quantum-mechanical character of a collision. In combination with advanced theoretical models, the experiments provide new knowledge on how a collision proceeds. I will give an overview of what we have learned so far, and how we can use our combination of techniques to study even more complex interactions.

6<sup>th</sup> December 2016, 11:35 – 11:55

#### *Bond-breaking and making on metal surfaces – a breakdown of the Born-Oppenheimer approximation?*

Paul Spiering (LEI), Joerg Meyer

Transition states are essential for chemical reactions on surfaces and consequently key for heterogeneous catalysis. Within the Born-Oppenheimer approximation (BOA), these special points along well-defined reactions paths determine reaction rates. Recent experiments[1] have further nurtured doubts about the BOA during chemical processes at metallic surfaces.[2]

The BOA is fundamental in state-of-the-art first-principles-based theory. In this work, we are going beyond the BOA by investigating the importance of non-adiabatic effects along for H<sub>2</sub> dissociation on Cu(111).

Building on electronic friction theory we have developed a new approach that allows us to systematically verify the accuracy of friction tensors.

[1] H. Ostrom et al., Science (2015)

[2] G.-J. Kroes, Science 321, 794 (2008)

6<sup>th</sup> December 2016, 11:55 – 12:15

#### *Multiphoton ionization and dissociation of rotationally warm, translationally cold CO via the B and E electronic states*

Zhongfa Sun (RU),

Carbon monoxide, CO, a key molecule in molecular dynamics, is usually detected by resonance enhanced multiphoton ionization (REMPI), which is highly efficient but has a disadvantage of fragmentation. We describe in this talk the mechanism of the C<sup>+</sup> and O<sup>+</sup> formation processes using Velocity Map Imaging technique under an unconventional pulsed beam geometry, which gives access to a wide range of initial states of CO. Previous assignments for these multiphoton processes via the CO B-state are improved and extensive studies for the E-state are carried out. The resonant enhancement effects on multiphoton dissociation processes of CO<sup>+</sup> are discussed in detail.



## Abstracts parallel lectures 6/7 December

### Room 55/57: Zeolites for catalysis

6<sup>th</sup> December 2016, 16:00 – 16:20

#### *Synergetic Effect of Lewis and Brønsted Acidity in Methanol to Olefins Reaction*

(TUD), Irina Yarulina<sup>1</sup>, Alexey Pustovarenko<sup>1</sup>, Javier Ruiz Martinez<sup>2</sup>, Bert M. Weckhuysen<sup>2</sup>, Klaartje Houben<sup>3</sup>, Mark Baldus<sup>3</sup>, Freek Kapteijn<sup>1</sup> and Jorge Gascon<sup>1</sup>

Modification of zeolite acidity with Ca leads to almost complete disappearance of Brønsted and the appearance of Lewis acidity. The synergetic effect of these two types of acid sites was studied in the methanol-to-olefins (MTO) reaction. The modification led to two times higher selectivity to propylene and nine times longer catalyst lifetime. Based on the catalytic performance and multiple characterization techniques it was concluded that decreased Brønsted acidity leads to increased propylene selectivity while Lewis acidity prolongs catalyst lifetime, both effects partially suppressing the aromatic cycle in the MTO mechanism.

6<sup>th</sup> December 2016, 16:20 – 16:40

#### *Stable performance of Mo/HZSM-5 in methane aromatization*

Nikolay Kosinov (TU/e), Ferdy Coumans, Emiel Hensen

Methane dehydroaromatization (MDA) over Mo/HZSM-5 catalysts is intensively investigated as a potential route to valorize natural gas. The main obstacle towards industrial application of this aromatics-producing reaction is rapid catalyst deactivation due to deposition of carbonaceous deposits; the low thermal stability of bifunctional Mo/HZSM-5 catalysts severely limits possibilities for regeneration by coke burn-off. In this work, we systematically studied the relation between structure (texture, Mo speciation, acidity) and stability of Mo/HZSM-5 catalysts. The new insights into the nature of the active phase and its stability against re-oxidation allowed designing catalysts and regeneration protocols that can withstand high-temperature reaction-regeneration cycles without significant loss of activity.

6<sup>th</sup> December 2016, 16:40 – 17:00

#### *Novel molecular recognition and confinement-driven reactivity concepts in zeolite catalysis for biomass valorization*

Roderigh Y. Rohling (TU/e), Evgeny Uslamin, Ionut Tranca, Emiel. J. M. Hensen, Evgeny A. Pidko

Conventional reactivity concepts in zeolite catalysis are centered around the intrinsic properties of individual sites promoting the catalytic transformations. In this work we show that such classical single-site reactivity models may not hold when catalysis in the pores of low-silica zeolites is considered. We carried out a comprehensive DFT study of the Diels-Alder cycloaddition/dehydration reaction between furanic compounds and alkenes over faujasite-type zeolites. This reaction represents a route to biomass-derived aromatics. Calculations demonstrate that molecular recognition features of zeolite nanocages define the possibility to establish the favorable reaction paths, while the specific chemistry of intrazeolite sites is much less important.

## Abstracts parallel lectures 6/7 December

### Boszaal: Transformations with Grignard reagents

6<sup>th</sup> December 2016, 16:00 – 16:20

#### *Catalytic asymmetric synthesis of chiral N-heterocyclic aromatic compounds*

Francesco Lanza (RUG), Ravi Jumde, Marieke Veenstra, Syuzanna R. Harutyunyan

The majority of all known active pharmaceutical ingredients (API) contain functionalized heterocyclic aromatic rings with a preponderance of N-containing aromatic heterocycles. Approximately half of all APIs are chiral molecules. Here, we describe our recent report in Science magazine on chemoselective catalytic asymmetric transformation of a wide range of  $\beta$ -substituted conjugated alkenyl-heteroaromatics to their corresponding chiral alkylated products. This operationally simple methodology makes use of copper-catalyzed addition of Grignard reagents and allows the introduction of both linear and branched, as well as functionalized alkyl chains and aryl groups at their  $\beta$ -carbon position.

6<sup>th</sup> December 2016, 16:20 – 16:40

#### *Functionalization of P<sub>4</sub> Using Lewis Acid Stabilized Bicyclo[1.1.0]tetraphosphabutane Anions*

Jaap E. Borger (VU), Andreas. W. Ehlers, J. Chris Sootweg, Koop Lammertsma

The direct functionalization of white phosphorus is an important target, which aims to avoid the use of  $\text{PCl}_3$  for the preparation of organophosphorus compounds. The high reactivity makes  $\text{P}_4$  unpredictable and to allow selective conversions, control is required.

A novel approach is the use of organolithium reagents. These C-nucleophiles can open up the  $\text{P}_4$ -cage, generating P-C bonds, but, often resulting in low selectivity and product mixtures. The first step is the scission of one P-P bond, generating transient bicyclo[1.1.0]tetraphosphabutanides. We will show our strategy to stabilize and isolate these reactive intermediates, and describe their reactivity pattern in subsequent controlled reactions.

6<sup>th</sup> December 2016, 16:40 – 17:00

#### *Chiral amides via catalytic asymmetric synthesis*

Xingchen Yan (RUG), M.C. Rodríguez Fernández, Syuzanna R. Harutyunyan

Although 1,4-additions of organometallics to conjugated enones, lactones, and esters is an established methodology, no progress has been seen in additions to conjugated amides despite their synthetic potential of the resulting  $\beta$ -substituted amides. The lower intrinsic reactivity of amides and the challenge to control the different conformers present in acyclic systems, are the main factors for paucity of methodologies.

We report the first asymmetric synthesis of enantiopure  $\beta$ -substituted amides via Lewis acid promoted copper-catalyzed addition of Grignards to low-reactive acyclic conjugated amides. Variety of amides with dialkyl, dibenzyl and diallyl substituents at N-atom can be employed using this methodology with excellent results.

## Abstracts parallel lectures 6/7 December

### Room 58: Process Intensification and Flow Chemistry – 2

6<sup>th</sup> December 2016, 16:00 – 16:20

#### *CONTINUOUS CHIRAL SEPARATIONS IN MICROREACTORS*

S. Susanti (RUG), Tim G. Meinds, Erik B. Pinxterhuis, Boelo Schuur, Johannes G. de Vries, Ben L. Feringa, Jozef G. M. Winkelman, Jun Yue, Hero J. Heeres

The potential of microreactors for enantioselective liquid-liquid extraction has been explored. The experiments were performed in capillary microreactors with combined reactive extraction and phase separation, for the chiral separation of a representative racemic amino acid derivative (3,5-R,S-DNB-Leu) dissolved in water by using a chiral host (a chinchona alkaloid) in the organic phase (1-octanol or 1,2-DCE). The results show that the ee is higher at short residence times of the two liquid phases in comparison with the ee at equilibrium. The performance and advantages of microreactor operation in chiral separation will be further discussed.

6<sup>th</sup> December 16:20 – 16:40

#### *Removal of Metal Ions from Water with Hydrophobic Deep Eutectic Solvents*

Dannie J.G.P. van Osch (TU/e), Dries Parmentier, Carin Dietz, Adriaan van den Bruinhorst, Maaïke C. Kroon, Remco Tuinier,

Deep eutectic solvents were used for the removal of metal ions from water. It was shown that the extraction occurs via an ion exchange mechanism in which all transition metals could be extracted with high distribution coefficients, even for high  $\text{Co}^{2+}$  concentrations and low mass fractions of DES. Maximum efficiency could be extracted within 5 s and regeneration was possible.

6<sup>th</sup> December 2016, 16:40 – 17:00

#### *Modeling an annular LED-based photocatalytic reactor for gas phase applications*

Maryam Khodadadian (TU/e),

An annular LED-based photocatalytic reactor was modelled by coupling a radiation field model with a reactor model. Toluene degradation was studied as the model reaction. We carried out validation experiments with varying inlet concentration, volumetric flow rate, irradiance and relative humidity. Model parameters were estimated by fitting the model predictions and experimental data using a least square method. The model predictions corresponded well to the experimental results. We conclude that the model can be used as an efficient tool for design, optimization and scale-up of LED-based photocatalytic reactors.

## Abstracts parallel lectures 6/7 December

### Parkzaal: Colloids

6<sup>th</sup> December 2016, 16:00 – 16:20

*Colloidal recycling: Reconfiguration of Random Aggregates into Patchy Particles*  
Vera Meester (LEI), Ruben Verweij, Casper van der Wel, Daniela J. Kraft

We present an approach for creating anisotropic patchy particles by reconfiguring randomly shaped aggregates of colloidal spheres. We achieve this reconfiguration of undesired random aggregates by depositing droplets of an apolar solvent at the contact points. The swelling lowers the attractive van der Waals forces, lubricates the contact area between the spheres, and drives the reorganization. This enables the synthesis of patchy particles with controlled and unprecedented patch arrangements. We demonstrate the broad applicability of this recycling strategy for making patchy particles as well as clusters of spheres by varying the swelling ratio, swelling solvent, surfactant concentration, and swelling time.

6<sup>th</sup> December 2016, 16:20 – 16:40

*Sculpting silica colloids by etching silica rods with non-uniform compositions*  
Fabian Hagemans (UU), Ernest B. van der Wee, Alfons van Blaaderen, Arnout Imhof

We present the shape transformation of rod-like silica rods by mild etching with NaOH in water, which were found to transform into cone shaped particles. The mechanism involves silica etching taking place with varying rate along the particle's length. Additionally, we show that etching rods where a silane coupling agent alone was incorporated and subsequently coupled to a fluorescent dye resulted in fluorescent silica cones, the orientation of which can be imaged using super-resolution confocal microscopy. Moreover, we show that it is possible to chemically manipulate the gradient and such prepare a particle containing segments that are more susceptible to etching.

6<sup>th</sup> December 2016, 16:40 – 17:00

*Tuning the phase diagram of colloid-polymer mixtures via additional soft colloidal interactions*  
Alvaro Gonzalez Garcia (TU/e), Remco Tuinier

Theory is presented to compute the phase diagram of Yukawa interacting spheres in a sea of polymeric depletants. It is found that additional Yukawa beyond hard core interactions strongly affect the locations of the coexistence regions. The theoretical phase diagrams are compared to Monte Carlo simulations, considering the depletion and the hardcore Yukawa pair potentials. The match between the two approaches validate the approximations. This opens up a way to predict the stability of realistic colloid-polymer mixtures.

## Abstracts parallel lectures 6/7 December

### Auditorium: Polymer Materials

6<sup>th</sup> December 2016, 16:00 – 16:20

#### *Structured amphiphilic and omniphobic materials for antifouling applications*

S. Kommeren (TU/e), T. Sullivan and C.W.M. Bastiaansen

Both amphiphilic and omniphobic materials have recently been considered as promising candidates for marine antifouling and fouling release applications. Creating systematically controllable surface relief in these materials is of potential interest for disruption of cell settlement and in lubricant retention on surfaces for instance. Furthermore, photochemically cross-linked (UV cured) high-performance films with such topography could have widespread practical applications. Here, we report novel methods of producing such surface structures and demonstrate that the shape of the produced surface relief can be altered by changing the processing conditions, including energy dose, monomer composition and the added solvent volumes. We provide novel examples of such materials, including structured hydrogels, fluorogels and amphiphilic networks, and discuss the application of these materials as practical antifouling materials.

6<sup>th</sup> December 2016, 16:20 – 16:40

#### *Strain-stiffening in synthetic hydrogels: Mimicking biological networks*

Marcos Fernandez Castano-Romera (TU/e), Rint P. Sijbesma

Soft biological tissues are characterized by a propensity to stiffen in response to large deformations that otherwise could threaten their integrity. Such complex mechanical behavior, absent in the vast majority of synthetic materials, is referred to as strain-stiffening and is shared by a number of network-forming fibrous proteins, including actin, collagen and intermediate filaments.

We have recently developed a synthetic system of semi-flexible rodlike micelles based on diacetylene bisurea bolaamphiphiles whose morphology can be fixated upon topochemical polymerization. Cross-linking of such rods leads to hydrogels exhibiting strain-stiffening with biologically relevant values and allows studying the underlying stiffening mechanisms.

6<sup>th</sup> December 2016, 16:40 – 17:00

#### *Polymer-templated chemical solution deposition of ordered multiferroic nanocomposites*

J. Xu (RUG), J. Varghese, J. A. Heuver, J. Momand, B. J. Kooi, B. Noheda, K. Loos

Multiferroic nanocomposites combine ferroelectric and ferromagnetic materials at the nanoscale. Various nanocomposite systems have demonstrated magnetoelectric coupling between the two ferroic phases, which makes them great candidates for applications such as four-state memory devices and magnetic field sensors. The previously studied multiferroic nanocomposites are predominately fabricated via physical vapor deposition, which requires expensive equipment and is unsuitable for large-scale manufacture. Here we present a low-cost chemical solution deposition approach for ordered structures of multiferroic nanocomposites, using patterned polymer thin films as templates. The multiferroic properties of the composites are demonstrated by electric and magnetic studies.



## Abstracts parallel lectures 6/7 December

### Room 82/83: 2-Dimensional Nanomaterials

6<sup>th</sup> December 2016, 16:00 – 16:20

#### *Nanographenes from (halo)bianthryls on Cu(111) and Au(111)*

P. H. Jacobse (UU), A. van den Hoogenband, M.-E. Moret, I. Swart, R. J. M. Klein Gebbink

Dibromobianthryl has been used as a precursor for the synthesis of armchair-type graphene nanoribbons via on-surface Ullmann coupling chemistry. Using scanning tunneling microscopy and atomic resolution atomic force microscopy, we study the coupling behaviour of the analogous dichlorobianthryl and non-halogenated bianthryl on Cu(111) and Au(111) and find that they give rise to various non-Ullmann coupled products. On copper we obtain CH bond activation at the C2 position to obtain 3,1-chiral nanoribbons, whereas on gold the dehalogenation and cyclodehydrogenation reactions are reversed to obtain oligobisanthenes.

6<sup>th</sup> December 2016, 16:20 – 16:40

#### *Self-assembly and on-surface polymerization of bromine-functionalized pyrene derivatives on noble metal surfaces*

Bay V. Tran (RUG), Tuan Anh Pham, Fei Song, Manh Thuong Nguyen, Milan Kivala and Meike Stöhr

In recent years, on-surface polymerization has been introduced as an alternative method to classical solution-based organic synthesis for constructing novel 1D and 2D materials. Here, we report on both the self-assembly and on-surface polymerization based on Ullmann coupling of bromine-functionalized pyrene derivatives on noble metal surfaces under ultrahigh vacuum (UHV) conditions [1]. For the formation of the polymer network we compared annealing in a hydrogen atmosphere to “normal” annealing in UHV whereas the hydrogen treatment resulted in improved polymer structures and cleaner surfaces [2].

[1] T.A. Pham et al., Chem. Eur. J., doi: 10.1002/chem.201504946

[2] B.V. Tran et al., in preparation

6<sup>th</sup> December 2016, 16:40 – 17:00

#### *Surfactant assisted synthesis of metal organic framework nanosheets. Applications in gas separation and chemical sensing.*

Alexey Pustovarenko (TUD), Beatriz Seoane, Maarten Goesten, Freek Kapteijn, Jorge Gascon

A new method for the synthesis of self standing 2D nanosheets of Al based metal organic frameworks is presented. We show that pre-organization of the Al building block and rapid mixing with the MOF linker result in the controlled synthesis of homogeneous nanosheets of non lamellar MOF structures. The application of the resulting self standing 2D solids in gas separation and chemical sensing will be thoroughly discussed.

## Abstracts parallel lectures 6/7 December

### Room 63/64: Light harvesting

6<sup>th</sup> December 2016, 16:00 – 16:20

#### *An Ab-initio Study of the Spectroscopic Properties of Solubilized LHCII*

P. López-Tarifa (VU), N. Liguori, R. Croce, L. Visscher

The major light-harvesting complex of photosystem II (LHCII) serves as the principal solar energy collector in the photosynthesis of green plants. Advances in X-ray diffraction and crystallization techniques have delivered LHCII structures at high resolution, although recent studies have shown that LHCII in the membrane does differ substantially from the crystal [Liguori et al., Sci. Rep. (2015)]. In this work, we apply Time-dependent Density Functional Theory (TD-DFT) in the linear response regime using the ADF code, to provide insights into how thermal conformational changes of the solubilized protein ligands affect the spectroscopic features of selected chromophores. P. López-Tarifa<sup>1</sup>, N. Liguori<sup>2</sup>, R. Croce<sup>2</sup> and L. Visscher<sup>1</sup>

<sup>1</sup> Amsterdam Center for Multiscale Modeling, Dep. Theoretical Chemistry, Faculty of Sciences, VU University Amsterdam, De Boelelaan 1083, 1081 HV Amsterdam, The Netherlands.  
<sup>2</sup> Laboratory of Biophysics of Photosynthesis, Dep. Physics and Astronomy, Faculty of Sciences, VU University Amsterdam, De Boelelaan 1083, 1081 HV Amsterdam, The Netherlands.

6<sup>th</sup> December 2016, 16:20 – 16:40

#### *Long-range exciton diffusion in perylene diimides mediated by singlet fission*

Kevin M. Felter (TUD), Valentina M. Caselli, T.J. Savenije, F.C. Grozema

The favorable electronic coupling and energetics of perylene diimides (PDIs) allow efficient singlet fission (SF) and triplet-triplet annihilation upconversion (UC) [1]. SF and UC influence the observed exciton diffusion length (L<sub>exc</sub>). This study aims to determine L<sub>exc</sub> in imid-substituted PDIs. Physical vapor deposited planar heterojunctions of crystalline Zinc Phthalocyanine (ZnPc) and PDI are studied by flash photolysis time resolved microwave photoconductance (FP-TRMC). FP-TRMC reveals L<sub>exc</sub> over tens of nanometers that can be correlated to efficient singlet fission. This initial result is valuable for the understanding of the role of singlet fission in excited state dynamics.

6<sup>th</sup> December 2016, 16:40 – 17:00

#### *In silico characterization of polymer-fullerene organic photovoltaic bulk heterojunctions*

Riccardo Alessandri (RUG), Alex H. de Vries, Remco W.A. Havenith, Siewert J. Marrink

In organic photovoltaic materials the charge separation process may be initiated by ultrafast electron transfer. The presently most efficient materials require a bulk heterojunction, an active layer composed of intimately intermixed electron acceptors and electron donors. The layer morphology has been shown to have a decisive impact on the charge separation.

Here multiscale modeling is used to investigate the morphologies and their impact on the charge separation. First, coarse-grain molecular dynamics models are used to generate morphologies, which are then back-mapped to atomistic resolution. Quantum chemical calculations are used to determine the electronic structure of bulk and interface molecules.

## Abstracts parallel lectures 6/7 December

### Room 65: Spectroscopy tracking of reactions

6<sup>th</sup> December 2016, 16:00 – 16:20

*Deamidation reactions of asparagine and glutamine containing peptides investigated by ion spectroscopy*  
Lisanne J.M. Kempkes (RU), Jonathan Martens, Josipa Grzetic, Giel Berden, Jos Oomens

For protonated peptides containing glutamine (Gln) and asparagine (Asn) residues, deamidation is a major fragmentation channel upon collision induced dissociation (CID) in mass spectrometry, competing with formation of sequence ions. We investigate NH<sub>3</sub>-loss reactions in terms of the product ion structures by infrared ion spectroscopy using the free electron laser FELIX and density functional theory (DFT). This study provides a comprehensive molecular structure map of the CID chemistry of the series of dipeptides AlaAsn, AsnAla, AlaGln and GlnAla, and indicates that while NH<sub>3</sub> is always detached from the residue, the reaction mechanisms for the four dipeptides are different.

6<sup>th</sup> December 2016, 16:20 – 16:40

*Benchmarking simulation protocols for the amide I spectra of proteins*  
Ana V. Cunha (RUG), Thomas L. C. Jansen

The amide I mode is widely used in IR spectroscopy of proteins due to the high sensitivity to secondary structure. Here, a benchmark of amide I spectral simulation protocols is presented, by comparing modeled FTIR and two-dimensional infrared (2DIR) spectra of three proteins with experimental data. The tested simulation protocols use all-atom molecular dynamics, combined with different electrostatic mappings/coupling models. This provides insight to the best choice of molecular dynamics force fields and spectral models for interpreting experiments. We found that FTIR spectra are accurately predicted by most models, while the 2DIR spectra are much more sensitive.

6<sup>th</sup> December 2016, 16:40 – 17:00

*Plasmon-enhanced fluorescence monitoring of a redox sensitive dye (methylene blue)*  
Martin Caldarola (LEI),

I will present our recent experiments towards the detection of the dynamics of redox reactions at single molecule (SM) level. We use a fluorescence readout for the redox potential, based on the redox sensitive dye Methylene Blue (MB), that is fluorescent in its oxidized state and turns dark when it is reduced. However, due to its low quantum yield of 4%, to enable single-molecule detection we need to enhance the fluorescence signal. To this aim we use individual gold nanorods that provide enhancement factors as large as 1000 and thus enable SM detection of MB molecules. With this enhancement scheme we aim to study the dynamics of redox reactions.

## Abstracts parallel lectures 6/7 December

### Room 55/57: Fischer-Tropsch Catalysis

6<sup>th</sup> December 2016, 16:00 – 16:20

*Gas phase propene epoxidation on gold: Catalyst design and mechanistic insight*  
Shamayita Kanungo (TU/e), M. Fernanda Neira D'Angelo

Gas phase epoxidation of propene to propene oxide (PO) in presence of H<sub>2</sub> and O<sub>2</sub> on Au-Ti catalysts is a greener alternative to commercially used processes for PO production, but hurdles like low conversion and H<sub>2</sub> efficiency have kept this process from replacing the traditional ones. In this study, silylation was used to enhance the performance of Au-Ti catalysts, which led to increased rates of PO formation, higher PO selectivity and H<sub>2</sub> efficiency. Different silylation techniques and agents were also explored. In addition, the role of the reducing gas was also studied using experiments and theoretical calculations (DFT).

6<sup>th</sup> December 2016, 16:20 – 16:40

*Porosity enhancement of niobia-supported cobalt catalysts for Fischer–Tropsch Synthesis*  
C. Hernández Mejía (UU), K.P. de Jong

Niobia-supported cobalt catalysts have gained considerable interest for Fischer–Tropsch Synthesis (FTS) due to their high selectivity towards long-chain hydrocarbons (C<sub>5</sub>+) and great activity per unit weight of cobalt. However, the crystal phase of niobia active for FTS has very low specific surface area and specific mesopore volume; limiting deposition of high cobalt loadings. The goal of this research is to increase the porosity of niobia by means of carbon deposition as structural template during crystallization. The resulting porous material was used as support for catalysts with higher cobalt loading. These catalysts showed high cobalt-specific catalytic activity and an important increase in C<sub>5</sub>+ selectivity.

6<sup>th</sup> December 2016, 16:40 – 17:00

*Progress in understanding iron-based Fischer-Tropsch catalysis for olefin synthesis*  
Manuel J. Louwerse (UU), Jingxiu Xie, Krijn P. de Jong

Iron-based Fischer-Tropsch catalysis is a way to produce light olefins from synthesis gas. However, obtaining good selectivity is not easy, since side-reactions towards coke, alkanes and especially methane are always present. Our group has and has had many projects on this subject, including studying promoter effects, particle size effects, and support effects. Techniques include colloidal preparation to control particle size, SSITKA experiments to study mechanistics, TEOM measurements to follow coke formation, and theory to understand promoter effects on the smallest scale as well as the balance between mechanistic steps on slightly larger scales. In this lecture, I will touch upon latest results from several of these projects.

## Abstracts parallel lectures 6/7 December

### Boszaal: Water oxidation

6<sup>th</sup> December 2016, 16:00 – 16:20

*In operando studies on molecular water oxidation catalysts*  
Cornelis J.M. van der Ham (LEI), Dennis G.H. Hetterscheid

Molecular iridium complexes show excellent activity in the water oxidation reaction, albeit the nature of the true active species is still under debate. In this contribution the water oxidation reaction mediated by molecular iridium catalysts is investigated by on-line characterization techniques including online electrochemical mass spectrometry and electrochemical quartz crystal microbalance studies. This allows us to determine the stability, activity and activation processes taking place as a function of time and applied potential. Depending on the structure of the (pre)catalysts and the reaction conditions the catalytic activity can be attributed to a molecular active species or iridium oxide nanoparticles.

6<sup>th</sup> December 2016, 16:20 – 16:40

*Solvent dependence of the formation of reactive non-heme intermediates with H<sub>2</sub>O<sub>2</sub>*  
Sandeep K. Padamati (RUG), Apparao Draksharapu, Duenpen Unjaroen, Wesley R. Browne

Understanding the formation and reactivity of non-heme Fe(III)-OOH and Fe(IV)=O complexes is of central importance to the study of non-heme iron dependent enzymes such as Tau-D and metallodrugs such as bleomycin. In this presentation we show that solvent and especially water content plays a crucial role in both the formation and reactivity of non-heme Fe(III)-OOH species with N<sub>4</sub> donor ligands. The formation and reactivity is studied by a combination of room and low temperature UV/vis absorption, EPR and resonance Raman spectroscopies and spectroelectrochemistry. Furthermore, the formation of stable Fe<sup>III</sup>-O-Fe<sup>III</sup> species is shown to be dependent on the water content.

6<sup>th</sup> December 2016

*A closed system approach to investigate the catalytic cycle of a copper water oxidation catalyst*  
Jessica M. de Ruiter (LEI), Francesco Buda

A deep understanding of the catalytic mechanism is a crucial step in the search for efficient homogeneous water oxidation catalysts (WOC) based on abundant transition metals. We introduce a computational strategy based on constrained ab-initio molecular dynamics to fully explore the key O-O bond formation reaction for the mononuclear copper WOC Cu(bpy)(OH)<sub>2</sub>. The novelty of the present approach is the inclusion of both proton and electron acceptors in the same simulation box. The explicit treatment of the solvent allows to determine the most likely catalytic cycle and provides a detailed view of the proton-coupled electron transfer process.

## Abstracts parallel lectures 6/7 December

### Room 58: Modelling of processes and Biomass Processing

6<sup>th</sup> December 2016, 16:00 – 16:20

*Effects of mass transfer and alkaline metals on the pyrolysis of cellulose*

R. Westerhof (UT), R. Westerhof

Pyrolysis could be an interesting technology to convert biomass into liquid fuels and / or chemicals. However, current liquid yields are moderate and chemicals are only present in (very) low concentrations. We have shown that under fast mass transfer conditions (removal and quenching rate of the products) high yields of sugars (70%) can be obtained from cellulose and that the molecular weight distribution of these sugars can be steered by the temperature. Results are presented that show the strong catalytic effect of alkaline and alkaline earth metals on the pyrolysis process.

6<sup>th</sup> December 2016, 16:20 – 16:40

*DNS for flow and heat transfer through random open-cell solid foams: Development of an IBM based CFD model*

Saurish Das (TU/e),

Open-cell solid foams are commonly used in chemical and process industries as a catalyst support. To simulate flow and heat transfer through such complex random solid structures, a sharp-interface Immersed Boundary Method (IBM) has been developed. A 3D image dataset from a Micro-CT scan of an actual foam geometry is usually converted into a surface-mesh of unstructured triangular elements and the current framework can embed it as an immersed boundary in a Cartesian CFD domain. The use of a Cartesian grid makes this method robust, computational friendly, and it avoids the tedious volumetric mesh generation process.

6<sup>th</sup> December 2016, 16:40 – 17:00

*Development of a continuous process for hydrothermal conversion of lignin*

Lara Truter (TU/e),

Lignin, a renewable aromatic compound, shows great potential for the production of industrially relevant aromatic bulk and fine chemicals. Recently, there have been various approaches in the conversion of lignin to well-defined aromatic compounds such as the hydrothermal depolymerization of lignin in a batch reactor [1]. For industrial implementation it is highly desirable to make this process continuous. This study focuses on the development of a continuous process for the hydrothermal conversion of lignin by investigating which reactor type and operating conditions would be most favourable. One reactor configuration investigated will be a multi-stage tubular reactor which operates at pH>12, 250 °C, 40 bar, using a Pd/C catalyst packed bed.

## Abstracts parallel lectures 6/7 December

### Parkzaal: Self-assembly

6<sup>th</sup> December 2016, 16:00 – 16:20

#### *Multiscale self-assembly of microtubes*

S. Ouhajji (UU), J. Landman, S. Prevost, A.P. Philipse, A.V. Petukhov

Mixtures of beta-cyclodextrin and sodium dodecyl sulfate form complexes in a 2:1 molar ratio at elevated temperatures. Upon cooling to room temperature these complexes self-assemble into hollow microtubes. By adding colloidal particles into the mixture colloid-in-tube assemblies are obtained after a heating/cooling cycle. Depending on the ratio of colloid-to-tube diameters various structures can be formed such as zigzag, zipper and helical sphere chains.

The self-assembly of this complex system was characterized by synchrotron SAXS, covering a total of three orders of magnitude of spatial scales. Furthermore, the response of this system to variations in temperature and concentration was probed.

6<sup>th</sup> December 2016, 16:20 – 16:40

#### *Self-assembled Supraparticles by Spherical Confinement*

Da Wang (UU),

Colloidal crystalline supraballs, spherical assemblies of size- and morphology- controlled nanoparticles, can exhibit many different interesting meta-materials properties. The colloidal crystalline supraparticles were created by crystallizing monodisperse spherical nano- and micron-sized colloids in slowly evaporating emulsion droplets. Experiments and computer simulations confirmed that even in the absence of attractions, icosahedral symmetry is entropically favored over the face-centered-cubic structure that is stable in the bulk. We extended the spherical confinement method to binary and anisotropic nanoparticle systems. To study how the structure of the more complex supraballs is affected by the spherical confinement, work is in progress by advanced electron microscopy techniques.

6<sup>th</sup> December 2016, 16:40 – 17:00

#### *Reversible encapsulation of large colloids by oppositely charged small colloids*

Yong Guo (UU), Willem K. Kegel

We report the first example of reversible encapsulation of micron-sized large colloids by oppositely charged submicron small colloids. The reversibility is achieved by introducing a pH-responsive layer onto the small colloids. The layer consists of a mixture of polyacrylic acid and polystyrene, and its influence on the encapsulation behavior of small colloids is studied as a function of the ionic strength and pH of the solvent. We observe reversible encapsulation of large colloids by small colloids upon cycling the pH. Furthermore, the surface coverage of the smaller colloids on the surface of the large colloids is tunable by pH. An explanation based on DLVO-theory is provided to further understand the reversible encapsulation mechanism.

## Abstracts parallel lectures 6/7 December

### Auditorium: Biobased Chemistry

6<sup>th</sup> December 2016, 16:00 – 16:20

*Structure-property relations of biobased polyesters from 1,4-butanediol-analogues and biobased diacids*  
Frits van der Klis (WUR), Rutger J. I. Knoop, Lambertus A. M. van den Broek, Jacco van Haveren, Daan S. van Es, Johannes H. Bitter

Here we present a systematic analysis of the structure-property-relations of a series of novel polyesters. Methyl-substituted analogues of 1,4-butanediol were investigated: 1,4-butanediol (0 x Me), 1,4-pentaandiol (1xMe) and 2,5-hexaandiol (2xMe). From these diols, three series of polyesters were prepared using the following diacids: succinic acid, adipic acid and furan-2,5-dicarboxylic acid (FDCA). We found that in all series the glass transition temperature (T<sub>g</sub>) increases with the number of Me-groups. All building blocks can be prepared from renewable resources, and the possibility to influence the T<sub>g</sub> inspires to develop novel (biobased)polyesters.

6<sup>th</sup> December 2016, 16:20 – 16:40

*Bio-based building block for polymer synthesis using advanced oxidation systems*  
Tim G. Meinds (RUG), Ibrahim Chaabane, Paolo P. Pescarmona, and Hero J. Heeres

Bio-based building blocks for polymer production are receiving worldwide research attention [1]. A well-known example is furan-2,5-dicarboxylic acid (FDCA), an alternative for phthalic acid for PET synthesis [2]. We here report our studies on the synthesis of a saturated version of FDCA (THFDCA) from 5-hydroxymethylfurfural (HMF) using a two-step approach. In the first step, HMF is reduced to tetrahydrofuran-2,5-dimethanol (THFDM) using Pd/Al<sub>2</sub>O<sub>3</sub> in close to quantitative yields as has been earlier reported by our group [3]. The second step involves an oxidation using a gold-based catalysts in combination with air towards tetrahydrofuran-2,5-dicarboxylic acid (THFDCA). This sequence of reactions was used to aim for higher overall yields for THFDCA than the one with FDCA as the intermediate. Results with a particular focus on the oxidation of THFDM will be reported in this contribution.

Literature

1. A. Gandini, T. M. Lacerda, A. J. F. Carvalho, E. Trovatti, Chem. Rev., 2016, 116, 1637-1669.
2. E. de Jong, M. A. Dam, L. Sipos, G.-J. M. Gruter, Biobased Monomers, Polymers and Materials, 2012, 1-13.
3. G. Bottari, A. J. Kumalaputri, K. K. Krawczyk, B. L. Feringa, H. J. Heeres, K. Barta, ChemSusChem, 2015, 8, 1323-1327.

6<sup>th</sup> December 2016, 16:40 – 17:00

*A New Tandem Catalytic Route to Renewable Aromatic Chemicals from Biobased Furanics*  
Homer Genuino (UU), Shanmugam Thiagarajan, Jan van der Waal, Ed de Jong, Jacco van Haveren, Daan van Es, Bert Weckhuysen and Pieter Bruijninx

Sugar-derived furanics are attractive alternative resources for renewable aromatics. Here, a novel route to such aromatics is presented, involving Diels-Alder (DA) addition, mild hydrogenation, and, finally, tandem catalytic aromatization with acidic zeolites and Pd/C as catalysts [1]. Surprisingly, the final aromatization step can also be conveniently run in the solid-phase, using only an mesoporous zeolite Y as catalyst [2]. Mechanistic insights will be presented as well as rules for catalyst design (i.e. variation in acidity, porosity, bifunctional catalysts). The newly developed route addresses the general challenge of retro-DA activity typically encountered in the synthesis of furanics-derived aromatics. The solid phase strategy furthermore greatly improves the green credentials of the route and is anticipated to be much more broadly applicable.  
[1] Thiagarajan, S., Genuino, H. C., et. al., ChemSusChem 8 (2015) 3052.  
[2] Thiagarajan, S., Genuino, H. C., et. al., Angew. Chem. Int. Ed. 128 (2016) 1390



## Abstracts parallel lectures 6/7 December

### Room 82/83: Molecular Materials

6<sup>th</sup> December 2016, 16:00 – 16:20

#### *Supramolecular Nano-Assemblies for Biomedical Diagnostic Applications*

Jan Bart ten Hove (*WUR*), Steven van Kesteren, Lisa Timmers, Junyou Wang, Aldrik H. Velders

Nanoparticles such as Quantum Dots and gold nanoparticles show unique, size-dependent properties that allow them to be used in sensing applications. We functionalize these nanoparticles with a dendrimeric supramolecular toolbox and use host-guest interactions to control the self-assembly and/or disassembly of these nanoparticles and nano-assemblies upon the introduction of an external stimulus, such as the presence of a biomarker.

6<sup>th</sup> December 2016, 16:20 – 16:40

#### *Designing supramolecular hydrogels functionalized with biopolymeric- and therapeutic additives for biomedical applications*

Willem Noteborn (*LEI*), Damy Zwagerman, Victorio Saez Talens, Chandan Maity, Alexander Kros, Jan van Esch, Rienk Eelkema, Roxanne Kieltyka

Supramolecular materials have numerous envisaged applications ranging from electronics to biomaterials, in which their specific non-covalent interactions make up for their dynamic and interesting character. However, controlling their structural and physicochemical properties remains challenging. Here we demonstrate the use of biopolymeric crosslinkers that can induce gelation pathway selection, influencing the mechanical properties of a low molecular weight gelator (LMWG) system. Furthermore, we show its potential as a versatile drug delivery platform through physical or chemical conjugation of a drug molecule based on its preparation method.

6<sup>th</sup> December 2016, 16:00 – 16:20

#### *Degradation and Preservation of Contemporary Photo-Works*

Evert B. Reijers (*UU*), Leonardus W. Jenneskens.

Contemporary photo-works consist of either a silver gelatine (black and white) photo or a chromogenic colour photo that is covered with, for example, decorative paints (alkyd-, acrylic-, etc.). These photo-works have been identified as art-objects and now represent important contributions to Dutch cultural heritage. Whereas photos are intrinsically susceptible to degradation by external influences, some of the photo-works possess an even shorter lifespan, rendering them unsuitable for expositions. Examples of unexpected observations include the occurrence of a metal-free efflorescence upon paint surfaces, preferential degradation of one of the photo-dyes under dark conditions and the occurrence of dye diffusion throughout a gelatine layer. The photographic gelatine layer appears to play a pivotal role in all these cases.

## Abstracts parallel lectures 6/7 December

### Room 80/81: Inorganic nanoparticles

6<sup>th</sup> December 2016, 16:00 – 16:20

*InP-based quantum dots: A good cadmium-free alternative?*

Elleke van Harten (UU), Celso de Mello Donegá and Andries Meijerink

Indium phosphide quantum dots (InP QDs) have attracted great interest as a promising alternative for Cd-based QDs, due to their size tunable emission and their low intrinsic toxicity. However, the synthesis of InP QDs with optical properties similar to those of (commercially applied) CdSe QDs is challenging. Here we report a new synthesis method for InP-based QDs with an efficient narrow band emission throughout the visible spectrum. Moreover, we can successfully coat these QDs with silica, while retaining the optical properties. These QD-silica particles are interesting for bio-imaging and lighting applications.

6<sup>th</sup> December 2016, 16:20 – 16:40

*Unravelling the synthesis mechanism of ligand-protected silver nanoclusters*

Marte van der Linden (UU), Pieter Glatzel, Andries Meijerink, Frank de Groot

Ligand-protected noble metal nanoclusters (ca 1 nm in size) represent a fascinating new class of materials. Due to their small size these clusters have properties not found in larger nanoparticles, such as luminescence and size-dependent stability. The latter allows us to make clusters with particular chemical compositions rather than size distributions. Using a one-pot synthesis, we prepare clusters of 29 Ag atoms, protected by 12 bidentate ligands. The clusters are remarkably monodisperse without any purification. Using EXAFS (extended x-ray absorption fine structure), we take the first steps towards elucidation of the synthesis mechanism of these clusters. The EXAFS results are analysed with DFT based electronic structure calculations.

6<sup>th</sup> December 2016, 16:40 – 17:00

*Gold quantum dot-decorated micelles for multimodal imaging and therapy*

Mathew T. Hembury (UU), Hamed Asadi, Wim E. Hennink, Tina Vermonden

Gold nanoparticles of less than 2 nm (gold quantum dots, AuQDs) exhibit distinctive optical and magnetic properties compared to larger gold nanoparticles. However, the obvious therapeutic and imaging potential of AuQDs has been undermined by their unfavorable biointeractions and lack of stability in aqueous solvents. Here, we present a simple synthetic pathway integrating AuQDs within thermosensitive polymeric micelles. These AuQD-decorated micelles are stable in aqueous solutions, do not elicit cell toxicity and preserve the attractive near-infrared photonics of AuQDs. This innovative material design based on the mutually beneficial interaction of gold and thermosensitive polymers shows promise towards combined therapy (photothermal and chemotherapy) and live imaging applications.

## Abstracts parallel lectures 6/7 December

### Room 63/64: Multiscale modeling

6<sup>th</sup> December 2016, 16:00 – 16:20

*Adaptive QM/MM: Current Limitations and Advances*

J. M Boereboom (UU), R. E. Bulo

High accuracy simulations of molecular systems containing solvents require adaptive Quantum Mechanics/Molecular Mechanics (QM/MM) simulations to reduce computational cost, while still accounting for the diffusivity of solvents. These simulations partition the system into three regions; active (QM), environment (MM), and a transition region (partial QM/MM character).

The interpolation necessary for the transition region can be done in two ways; non-Hamiltonian (force interpolation), and Hamiltonian (energy interpolation). I will present the limitations of the non-Hamiltonian simulations (no energy conservation), and the challenges in developing a Hamiltonian approach. Finally, I will introduce the first Hamiltonian approach that properly describes an aqueous solution.

6<sup>th</sup> December 2016, 16:20 – 16:40

*Reactive trajectories of the Ru2+/3+ electron transfer reaction and the connection to Marcus' theory*

Ambuj Tiwari (UvA), Bernd Ensing

Outer sphere electron transfer between two ions in aqueous solution is a rare event on the time scale of first principles molecular dynamics simulations. We use transition path sampling to generate an ensemble of reactive trajectories of the self-exchange reaction between a pair of Ru2+ and Ru3+ ions in water. After aligning the trajectories with respect to the moment of barrier crossing, we can compute statistical averages over the path ensemble. We discovered that the outer sphere electron transfer between the metal ions is coupled to a proton transfer between their coordination shells.

6<sup>th</sup> December 2016, 16:40 – 17:00

*A systematic approach to calibrate a transferable force field parameter set*

Koen M. Visscher (VU),

In this work parameters are developed for a polarizable biomolecular force field. Starting from the non-polarizable GROMOS 53A5/53A6 parameter set, condensed-phase interaction parameters are calibrated using a QM/MM approach. Here we show that the transferability of force-field parameters can be improved by a systematic (analytical) approach to the calibration effort. Application of these approaches is demonstrated in the calibration of force-field parameter sets for small organic molecules, optimized to reproduce pure-liquid (thermodynamic, dielectric and transport) properties, as well as hydration free energies.

## Abstracts parallel lectures 6/7 December

### Room 65: Fast spectroscopy

6<sup>th</sup> December 2016, 16:00 – 16:20

#### *Extreme ultraviolet photoreactions of tin oxo cages*

Yu Zhang (UvA), Jarich Haitjema, Niklas Ottosson, Fred Brouwer

Molecular inorganic photoresists are considered for Extreme Ultra Violet lithography (EUVL) due to their strong photon absorption and small building block size, which allow high resolution and low line edge roughness. We will discuss EUV, DUV and e-beam reactivity of tin cages ( $[(\text{RSn})_{12}\text{O}_{14}(\text{OH})_6]\text{X}_2$ ) (R = organic group; X = anion). We use spectroscopic methods to obtain insight in the radiation induced changes. Once we understand the chemical reaction mechanisms we can propose rational strategies to improve the sensitivity and resolution of EUV photoresists. Such improvements are urgently needed to meet the demands of the semi-conductor industry.

6<sup>th</sup> December 2016, 16:20 – 16:40

#### *Ultrafast Dynamics of Electron-Hole Pairs in Ultrathin 2D InSe Layers*

Jannika D. Lauth (TUD), Frank C. M. Spoor, Aditya Kulkarni, Arjan J. Houtepen, Juleon M. Schins, Sachin Kinge,\* Laurens D. A. Siebbeles

2D semiconductors exhibit interesting dimensionality-dependent properties and bear high potential for ultrathin electronics. InSe has moved into focus as high mobility FET and high responsivity photodetector. We synthesized atomically thin InSe layers (1.7 nm, inaccessible by exfoliation) by colloidal methods and have fully characterized the 2D crystals with T/SEM, AFM, XPS and GISAXS[1]. With transient absorption spectroscopy, we evaluate the charge carrier dynamics in InSe layers and extract mobilities of  $\sim 30 \text{ cm}^2/\text{Vs}$  by applying terahertz spectroscopy. The combination of colloidal synthesis and ultrafast spectroscopy is a powerful tool for assessing the potential of 2D InSe for next generation electronics.

6<sup>th</sup> December 2016, 16:40 – 17:00

#### *Spectral Watermarking in Femtosecond Stimulated Raman spectroscopy: resolving the nature of the carotenoid $S^*$ state*

Miroslav Klotz (VU), Joern Weissenborn, Tomas Polivka, Harry A. Frank, John T.M. Kennis

A new method for recording femtosecond stimulated Raman spectra (FSRS) was developed that dramatically improves and automatizes baseline problems that in the past have notoriously obstructed the applicability of this technique. The experiment involves shaping of a broadband source, which allows locking the signal into watermarks that can be recovered from data with high fidelity. Through unique properties of Raman scattering, stimulated Raman signals with robust rejection of baselines and fixed-pattern-noise are obtained. The delivered improvement in FSRS was demonstrated by showing that the so-called  $S^*$  state of carotenoids corresponds to the optically forbidden  $S_1$  state of a sparsely populated carotenoid conformation.

## Abstracts parallel lectures 6/7 December

### Room 55-57: Catalytic organic synthesis

7<sup>th</sup> December 2016, 09:05 – 09:25

#### *Activation of an organocatalyst by a chemical signal*

Fanny Trausel (TUD), Chandan Maity, Jos M. Poolman, Davey S. J. Kouwenberg, Frank Versluis, Antonio M. Grande, Jan H. van Esch, Rienk Eelkema

Nature often uses enzyme activation to respond to chemical signals through signal transduction pathways. Such processes are unknown in synthetic materials. Here, we present a protected organocatalyst that is activated by reaction with a chemical signal. Such a catalyst allows autonomous response of a material to changes in its environment. Using self-immolative chemistry, we designed a protected aniline catalyst for hydrazone formation, where, upon activation of the pro-catalyst using hydrogen peroxide as a signal, the reaction rate increases 7-fold almost instantly. This system allows autonomous temporal control over the formation of polymer gels.

7<sup>th</sup> December 2016, 09:25 – 09:45

#### *Discovery and engineering of robust Baeyer-Villiger monooxygenases*

Elvira Romero (RUG), Max J.L.J. Fürst, Marco W. Fraaije

Baeyer-Villiger monooxygenases (BVMOs) can be used as biocatalysts for various selective oxidation reactions. However, most of the known BVMOs are rather labile enzymes. By genome mining and enzyme engineering, we have created a set of novel and robust BVMOs that display attractive biocatalytic features. Except for establishing their biocatalytic potential (for example for the efficient synthesis of various polymer precursors), we have also obtained valuable new insights into the mechanistic and structural properties of these oxidative biocatalysts through elucidation of crystal structure and pre-steady state kinetic analysis.

## Abstracts parallel lectures 6/7 December

### Room 58: Proton reduction catalysis

7<sup>th</sup> December 2016, 09:05 – 09:25

*An [FeFe]-hydrogenase mimic with an electron reservoir for efficient proton reduction in aqueous media*  
René Becker (UvA), Saeed Amirjalayer, Ping Li, Sander Woutersen, Joost N.H. Reek

Efficient hydrogen-generation catalysts are essential for realizing a hydrogen-based economy. Synthetic mimics of the hydrogenase enzyme are promising candidates, but are generally inefficient and oxygen sensitive. Here, we report on a synthetic hydrogenase mimic that operates in aqueous solution, is oxygen-tolerant, and displays high turnover number and frequency. The catalyst contains a redox-active phosphole ligand as an electron reservoir, a feature that is also crucial for the working of the natural enzyme. Using spectro-electrochemistry and time-resolved spectroscopy, we find that the electron reservoir actively partakes in the proton reduction and that its electron-rich redox states are stabilized through ligand protonation.

7<sup>th</sup> December 2016, 09:25 – 09:45

*Syntheses, Structures, and Electrocatalytic Hydrogen Production of N-Functionalized Ni-NHC Complexes*  
Siyuan Luo (LEI), Elisabeth Bouwman

Although Ni-NHC complexes have found various applications in organometallic chemistry, the electrocatalytic properties of this kind of compounds so far have been mostly neglected by researchers working in the field of organocatalysis. The handful of publications related to proton reduction with metal-NHC compounds mainly addressed cobalt-NHC complexes. With the aim to develop new electrocatalysts for proton reduction, several novel pyridine-functionalized NHC-Ni complexes have been synthesized, which were characterized by various methods. The synthesis and structures of the compounds, as well as their redox properties and electrocatalytic activity for proton reduction in organic solvent will be reported.

## Abstracts parallel lectures 6/7 December

### Room 65: Glasses

7<sup>th</sup> December 2016, 09:05 – 09:25

#### *Vitrification as a dynamical connectivity transition*

Ruben Higler (WUR), Jasper van der Gucht, Joris Sprakel

The quest to unravel the nature of the glass transition, where the liquid viscosity increases by many orders-of-magnitude, while its static structure remains largely unaffected, remains unresolved. Whereas various structural and dynamical precursors to vitrification have been identified, a predictive and quantitative description of how subtle changes at the microscopic scale give rise to the steep growth of macroscopic viscosity is missing. Here we explore how rigidity emerges in liquids of colloids as they vitrify. Combining experiments and theory, we arrive at a quantitative and parameter-free description of vitrification as a dynamical connectivity transition.

7<sup>th</sup> December 2016, 09:25 – 09:45

#### *Linking particle dynamics to local connectivity in colloidal gels*

Jan Maarten van Doorn (WUR), Joris Sprakel

Colloidal gels are a prototypical example of a heterogeneous solid whose complex properties are governed by thermally-activated dynamics. Understanding their properties remains challenging due to the strong heterogeneity in bonding structures at the local scale. In this Letter we study the connection between the intermittent dynamics of individual particles and their local degree of connectivity, using quantitative three-dimensional microscopy. We interpret our experiments by deriving a model that describes single-particle dynamics based on highly cooperative thermal debonding. The model, which is in quantitative agreement with our experimental data, provides a microscopic picture for the structural origin of dynamical heterogeneity in colloidal gels and sheds new light on the link between structure and the complex mechanics of heterogeneous solids.

## Abstracts parallel lectures 6/7 December

### Parkzaal: Protein-peptides

7<sup>th</sup> December 2016, 09:05 – 09:25

#### *Proteins in complex coacervates*

Saskia Lindhoud (UT), Mireille M.M.A.E. Claessens

Complex coacervates are liquid-like phases which form upon mixing oppositely charged macromolecule at the right pH, ionic strength and mixing ratio. Many protein/RNA droplets that are present in the cytosol have the same phase behaviour as complex coacervates. The central question of this research is whether complex coacervates can be used as a model system of the cytosol and/or protein droplets in the cytosol. We therefore study how many proteins can be incorporated in complex coacervates, whether the proteins remain biologically active, can aggregate and diffuse through these dense polymeric phases.

7<sup>th</sup> December 2016, 09:25 – 09:45

#### *Site-selective crosslinking of biomimetic hydrogels: Tuning gel mechanics without changing the architecture*

Daniel Schoenmakers (RU), Paul Kowar

Fibrous network gels support the intra- and extracellular environment of eukaryotes. Key aspects of these networks are mechanical stability, an architecture of bundles, and non-linear mechanical response to stress. Polyisocyanide (PIC)-based hydrogels uniquely mimic the architecture and the linear and nonlinear mechanical response of the natural materials. The mechanics of the PIC gels, however, slowly change over time (days). We developed a crosslinking approach to stabilize the PIC gels without changing its architecture. As a result, the mechanical properties become nearly temperature independent. We will also show which additional mechanical features the crosslinking approach introduces in these soft materials.



## Abstracts parallel lectures 6/7 December

### Auditorium: Catalysis

7<sup>th</sup> December 2016, 09:05 – 09:25

#### *Supported Silver Catalysts for Ethylene Epoxidation*

J.E. van den Reijen (UU), S. Kanungo, T.A. Nijhuis, K.P. de Jong, P.E. de Jongh

Ethylene epoxidation is a major industrial process with an annual world wide production in the millions of tons. This industrial process is based on  $\alpha$ -alumina supported silver particles with many additives to boost performance. We use model catalysts to show the influence of the support characteristics on the catalytic performance and stability. The model catalysts performs comparable to the industrial catalysts, but allow fundamental studies of particle size and surface effects.

7<sup>th</sup> December 2016, 09:25 – 09:45

#### *UV-Vis/DFT Study on Activation of Zirconocene Species in Zr/MAO/SiO<sub>2</sub> Polymerization Catalysts*

Marjolein E.Z. Velthoen (UU), Jelle M. Boereboom, Abdelkbir Bouhmadi, Michaël Cecius, Steve Diefenbach, Florian Meirer, Bert M. Weckhuysen

The molecular structures of bis(1-methyl-3-butylcyclopentadienyl)-based zirconocene, known to be present in SiO<sub>2</sub>/MAO/Zr polymerization catalysts, were studied with UV-Vis spectroscopy and DFT calculations. The simulated UV-Vis spectra of seven hypothetical zirconocene structures were compared with the experimental UV-Vis spectra of the catalyst materials under study. A new activation mechanism is proposed in which zirconocene activation proceeds through complexation with AlMe<sub>2</sub><sup>+</sup> species inherent to MAO, followed by internal exchange of ligands resulting in the release of TMA and the active cationic mono-methylated zirconocene. In accordance with the catalytic performance, an increase in MAO loading resulted in a higher number of active zirconocene species.

## Abstracts parallel lectures 6/7 December

### Room 82/83: Molecular crystals

7<sup>th</sup> December 2016, 09:05 – 09:25

#### *Understanding the solid-state phase transitions in molecular crystals*

Mireille Smets (RU), Sander Brugman, Ernst van Eck, Hugo Meekes, Herma M. Cuppen

To improve the shelf-life of polymorphic forms of active pharmaceutical ingredients, solid-state phase transitions in these materials should be prohibited. This research aims at understanding the mechanisms involved in transitions in molecular crystals, since established theories cannot fully explain all phenomena for this class of materials.

We present the in-situ characterization of phase transitions in linear amino acids, using various complementary techniques. We have previously shown that DL-norleucine exhibits cooperative motion during at least one of its transitions. Our current findings reinforce that the existing theory of phase transitions should be elaborated by incorporating the role of cooperative motion.

7<sup>th</sup> December 2016, 09:25 – 09:45

#### *Attrition enhanced deracemization of chiral sulfoxides*

Anthonius H. J. Engwerda (RU), Niels Koning, Paul Tinnemans, Hugo Meekes, F. Matthias Bickelhaupt, Floris P. J. T. Rutjes and Elias Vlieg

Despite the importance of enantiopure chiral sulfoxides, few methods exist that allow for its deracemization. Here, we show that enantiopure sulfoxides can be produced using Viedma ripening. In the Viedma ripening process, vigorous grinding of a slurry of chiral crystals in a saturated solution is combined with racemization in solution, which can result in complete solid phase deracemization. We report a series of 14 new crystal structures, from which one candidate suitable candidate for Viedma ripening was identified. Starting from a near or completely racemic mixture of this sulfoxide, Viedma ripening allowed for complete deracemization in combination with an excellent yield.

## Abstracts parallel lectures 6/7 December

### Room 80/81: Electrochemistry

7<sup>th</sup> December 2016, 09:05 – 09:25

*Reducing adsorption in nanochannels; from fundamental understanding to practical application*  
Hanan Al-Kutubi (RUG), Klaus Mathwig

Electrochemical nanofluidic devices are chip-based sensors consisting of a nanochannel of approximately 100 nm in height. By employing a pair of electrodes positioned at the top and bottom of this channel, the detected current can be greatly amplified, allowing much higher sensitivity and the possibility to investigate systems at the fundamental level. However, a high surface-to-volume ratio means that these channels suffer from adsorption of molecules onto the electrodes causing reduction in current and complication of experiments. By using additives, the absorptivity inside these nanochannels has been investigated with the aim of both understanding and reducing its effects.

7<sup>th</sup> December 2016, 09:25 – 09:45

*The mechanism of photocharging effect in BiVO<sub>4</sub> photoanodes: an in-situ study*  
Bartek J. Trzeźniewski (NWO), Tetsuro Nagaki, Isaac Herraiz-Cardona, Sandheep P. Ravishankar, David A. Vermaas, Ibadillah A. Digdaya, Alessandro Longo, Wim Bras, Sixto Gimenez, Wilson A. Smith

We elaborate on the possible mechanisms of PC in BiVO<sub>4</sub> photoanodes, and how it directly leads to improved Photo Electron Chemical (PEC) performance in the context of the Solar Light Junction, to provide further insights into the chemical and physical mechanisms behind the PC phenomenon. We use electrochemical impedance spectroscopy to investigate the effect of PC on the electronic properties of BiVO<sub>4</sub> and in-situ electrochemical X-ray absorption spectroscopy (XAS) to study the structural properties of BiVO<sub>4</sub> under PEC conditions. Our findings suggest that neither applying bias potential nor the photocharging treatment alters the chemistry of our BiVO<sub>4</sub> films.

## Abstracts parallel lectures 6/7 December

### Room 63/64: NMR Spectroscopy

7<sup>th</sup> December 2016, 09:05 – 09:25

#### *MicroMAS NMR - Enhanced Resolution and Sensitivity combining Homonuclear Decoupling and Inverse Detection*

J. Ole Brauckmann (RU), J.W.G. (Hans) Janssen, Ernst R. H. van Eck, Arno P.M. Kentgens

We developed a high-field (20 T) triple-channel micro magic angle spinning probe for solid-state NMR experiments. The proton resolution (0.14 ppm) is more than two times better than the result published in the literature so far. This opens the way for highly sensitive experiments using inverse detection of heteronuclei via protons employing homonuclear decoupling. We demonstrate that this combination is efficient at moderate spinning speeds and results in 5 times higher sensitivity for <sup>1</sup>H-<sup>13</sup>C correlations and <sup>13</sup>C-<sup>15</sup>N correlations. It even makes correlation spectroscopy of (~50) nanoliter sample volumes possible in natural abundance, thus providing a powerful tool for mass-limited samples.

7<sup>th</sup> December 2016, 09:05 – 09:45

#### *in situ probed solid-state NMR on photosynthetic thylakoid membranes*

Fatemeh Azadi (LEI), Giorgio Perrin, Karthick Babu Sai Sankar Gupta, Diana Simionata, Tomas Morosinotto, Anjali Pandit

Regulation in photosynthesis involves interplay between thylakoid membrane phase transitions and supramolecular re-arrangements of photosystems and light-harvesting proteins, and atomistic pigment and protein conformational changes. We present NMR data recorded in situ of U-<sup>13</sup>C-<sup>15</sup>N *Chlamydomonas reinhardtii* (Cr.) thylakoid membranes using polarization transfer spectral editing and T1ρ relaxation spectroscopy to follow protein and lipid molecular dynamics in intact photosynthetic membranes. A comparison of wild type and photoprotective Cr. mutants (npq2) reveals that npq2 membranes have altered protein and lipid dynamics properties, demonstrating the ability of in situ NMR for structure-functional characterization.

## Abstracts parallel lectures 6/7 December

### Boszaal: Astrochemistry

7<sup>th</sup> December 2016, 09:05 – 09:25

#### *B-DNA Stability and Replication in Non-Terran Bio-Solvents*

Trevor A. Hamlin (VU), Célia Fonseca Guerra, Jordi Poater, F. Matthias Bickelhaupt

We have computationally analyzed a comprehensive series of Watson-Crick, mismatched, and artificial B-DNA base pairs, in the gas phase and in several solvents, using dispersion-corrected density functional theory (DFT-D3). Our analyses shed light on how the molecular-recognition machinery behind life's genetic code depends on the medium, in order to contribute to our understanding of the possibility or impossibility for life to exist on exoplanetary bodies. In addition, the archetypical nucleophilic substitution at phosphorus has been examined in the same solvents. The topology of the potential energy surface is largely dependent on solvent polarity.

7<sup>th</sup> December 2016, 09:25 – 09:45

#### *High resolution infrared spectroscopy of molecular radicals of astrophysical interest / Solid state pathways towards molecular complexity in space*

Kirstin D. Doney (UL)

While the interstellar medium is dominated by hydrogen and helium, with only trace amounts of oxygen, nitrogen, and carbon, the majority of observed molecules are hydrocarbon or hydrocarbon derivatives. A better understanding of the spectroscopy associated with hydrocarbons can help determine which molecules are in particular astronomical environments and the chemical processes that occur there. Here we present high-resolution infrared results of gas-phase transients, like c-C<sub>3</sub>H<sub>3</sub><sup>+</sup> (the smallest aromatic molecule) and poly-acetylene chains, using cw-CRDS and supersonic planar plasma expansions. The resulting spectroscopic constants are needed as input for astronomical surveys or to interpret existing astronomical spectra.

## Plenary lectures and focus sessions 7 December

### Plenary lectures

#### Beneluxzaal

7<sup>th</sup> December 2016, 10:15 – 11:00

*Plenary lecture: Computational Chemistry from reactivity to NMR calculations*

Odile Eisenstein

Computational chemistry is currently used for determining reaction mechanisms and physical properties of chemical systems. While there is a tendency for representing the experimental systems as accurately as possible and for using computational methods that represent strong and weak interactions as precisely as possible, there is also room for trying to determine trends by considering simplified systems that carry the physics of the problem. Questions of the same nature apply for the calculations of physical properties, which are here the NMR chemical shifts.

We will use the d<sup>0</sup> olefin metathesis catalysts of the type M(X)(Y)(ER)(CHR) with M = Mo, W and ER = amido; M = Re and ER = alkylidyne, X, Y = C-, N-, O- anionic ligands. The influence of the ligands and the metal on the efficiency of the catalysis will be presented.[1]

The solid state NMR chemical shifts of the alkylidene <sup>13</sup>C for M(X)(Y)(ER)(CHR) with M = Mo, W and ER = amido; M = Re and ER = alkylidyne, M = Ta and ER = alkyl, X, Y = C-, N-, O- anionic ligands were determined by experiment, illustrating the anisotropy of the electronic environment of the alkylidene carbon in the various systems.[2] State-of-the-art fully relativistic 4 components (4c) calculations of the <sup>13</sup>C chemical shift tensor reproduce well the experimental values. Calculations show the absence of correlation between the <sup>13</sup>C isotropic chemical shifts and NBO charge of the alkylidene carbon. However, an NBO based analysis (Natural Chemical Shift) of the shape and directions of the shielding tensors calculated with 2 components calculations (validated by comparison with 4c calculations) provide a rationale of the observed values and demonstrate the role of the paramagnetic contributions in determining the chemical shifts.[3] If time permits, results concerning other systems such as metallacyclobutane which are intermediates in the olefin metathesis pathway will be presented.

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7<sup>th</sup> December 2016, 11:00 – 11:30

*KNCV Gold Medal lecture: Catalytic enantioselective synthesis of functional molecules: control over selectivity and reactivity*

Syuzanna Harutyunyan

Our research program is aimed at the development of novel catalysis concepts for the asymmetric synthesis of chiral functional molecules. In 2011 we introduced an entirely new role for Cu(I)-based catalysts, facilitating highly enantioselective carbon-carbon bond forming reactions between organometallics and enolisable carbonyl as well as imine compounds. Following this initial discovery, we established Cu(I)-catalysis, in combination with Lewis acids/Grignard reagent, as a powerful tool to tackle the reactivity of inherently unreactive substrates for carbon-carbon bond forming reactions. In this lecture I will focus on how we can use these concepts to access highly demanded and valuable chiral heteroarenes and amides, as well as tertiary alcohols and amines, in catalytic and enantioselective fashion.

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## Plenary lectures and focus sessions 7 December

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7<sup>th</sup> December 11:30 – 12:15

*Plenary lecture: Necessity is the Mother of Invention: Natural Products and the Chemistry they Inspire*  
Sarah Reisman

The chemical synthesis of natural products provides an exciting platform from which to conduct fundamental research in chemistry and biology. We are currently focused on devising concise approaches to polycyclic natural products such as ryanodol, acutumine, and psiguadial B. The densely packed arrays of heteroatoms and stereogenic centers that constitute these polycyclic targets challenge the limits of current technology and inspire the development of new synthetic strategies and tactics. This seminar will describe our latest progress in both our methodological and target-directed synthesis endeavors.

7<sup>th</sup> December 2016, 15:55 – 16:40

*Plenary lecture: Nanoscience Lives Here: Molecules, Materials, & Mechanisms*  
Jillian Buriak

Interfacing molecules with silicon is of enormous interest for applications in molecular electronics, for passivation of the surface, for integration of silicon devices with tissues, and further miniaturization of feature sizes of transistors on silicon into the sub-10 nm regime. The formation of silicon-carbon bonds is a practical and commonly used approach to chemically functionalize the surface of silicon due to the stability of the Si-C bond, and the surprisingly diverse number of distinct mechanisms, and hence reaction conditions, that can be harnessed to enable this chemistry. For instance, illumination of a hydrogen-terminated silicon surface in the presence of an alkyne or alkene was, at least initially, expected to proceed via a radical mechanism, in much the same manner as silicon-based molecules (silanes, R<sub>3</sub>Si-H for instance). Research over the past decade has shown, however, that the mechanisms in operation are far more diverse, and the chemistry much richer, than ever thought. The underlying electronics of the silicon play an important role in enabling the chemistry of the surface, and under many circumstances, can dominate. In this talk, we will discuss the latest developments in the surface chemistry of silicon that provide practical avenues for exquisitely precise integration of molecules with silicon surfaces. We will introduce the use of surface plasmons to drive new mechanisms that have no equivalent in molecular chemistry, and show how patterned plasmonic arrays enable nanopatterning via this chemical approach. The 'materials-only' plasmonic mechanism will be contrasted with new chemistry on silicon that enables the bonding of molecules via exotic chalcogenides (such as Si-S, Si-Se, Si-Te bonds), chemistry that is derived directly from the molecular literature. The case of silicon will be used to show the connection that is nanoscience, the bridge between materials and molecules.

7<sup>th</sup> December 2016, 16:40 – 17:25

*Plenary lecture: Mechanistic studies of Folding upon Binding*  
Jane Clarke

Many key protein-protein interactions are driven by assembly of complexes where one or both partner proteins are intrinsically disordered before binding. In this case the free energy of binding has to compensate for the energetic cost of folding. We are comparing the folding of a number of different

## Plenary lectures and focus sessions 7 December

folding-upon binding systems to ask some fundamental questions about the mechanisms of folding upon binding: What is the importance of residual structure? What role does the ordered partner play? What is the mechanism of assembly? And, perhaps most fundamentally – what is the function of disorder? I will describe some of our recent findings.

7<sup>th</sup> December 13:20 – 13:50

### **Lecture by our sponsor VO Patents**

Applying for financial grants and patents

Henri van Kalker (VO Patents) and Bram van Weerdenburg (Subsidiebureau Hezelburcht)

Patenting inventions and applying for financial grants to continue research and development often work synergistically. This not only applies to research in business environments, but also to academic settings. In this joined lecture between V.O. Patents & Trademarks and Hezelburcht, some basic insights with regard to intellectual property and the application of grants will be provided. In addition, the mutual strengthening of these aspects will be highlighted by some case studies that will demonstrate how you may profit from financial grants when applying for patents and vice versa.



## Plenary lectures and focus sessions 7 December

### Focus sessions

#### **Focus session: Activity-based protein profiling creates novel opportunities in drug discovery**

Chair: Kim Bonger

In the past decade, activity-based protein profiling has emerged as a powerful chemical biological strategy to investigate the biological function of enzymes in cells, tissues or animals. Activity-based labelling using chemical probes enables the assessment of the activity and inhibition of multiple endogenous enzymes providing novel research opportunities, including inhibitor discovery. In this focus session we highlight the recent developments in probe design and its applications in drug discovery research.

Lectures:

1. Ed Tate (Imperial College)

2. Paul Geurink (NKI; Ovaa)

*Diubiquitin FRET probes to quantify ubiquitin linkage specificity of deubiquitinases*

Deubiquitinating enzymes (DUBs) are proteases that fulfill crucial roles in the ubiquitin (Ub) system, by deconjugation of Ub from its targets and disassembly of polyUb chains. The specificity of a DUB towards one of the polyUb chain linkages largely determines the ultimate signaling function. We present a novel set of diubiquitin FRET probes, comprising all seven isopeptide linkages and equipped with Rhodamine110 and tetramethylrhodamine, for the absolute quantification of chain cleavage specificity by means of Michaelis–Menten kinetics. We demonstrate the value of our probes in the elucidation of the Lys11 specificity of the OTU DUB Cezanne.

3. Martijn Verdoes (RUMC)

*Quenched fluorescent cysteine cathepsin probes: tumor imaging and immunotherapy*

Cysteine cathepsins (CCTS) are proteases that play important roles in both normal physiology and many human diseases. In cancer, CCTS are upregulated and can be exploited for tumor imaging. We developed quenched activity-based probes (qABP) to study CCTS activity in living cells and organisms. We use these qABPs for noninvasive and multiphoton intravital imaging of mouse models of cancer and found that within the tumor microenvironment a subpopulation of macrophages with a pro-tumor phenotype are the major source of CCTS activity. We are currently investigating the functional characterization of this subpopulation of tumor resident macrophages, as well as designing molecules to manipulate these cells in vivo to advance cancer immunotherapy.

4. Hui Deng (LEI; Van der Stelt)

*Discovery of Chemical Probes to Study Brain Lipid Signaling*

Hui Deng (LEI), Daisuke Ogasawara, Andreu Viader, Marc P. Baggelaar, Arjen C. Breman, Hans den Dulk, Adrianus M.C.H. van den Nieuwendijk, Marjolein Soethoudt, Tom van der Wel, Juan Zhou, Hermen S. Overkleeft, Manuel Sanchez-Alavez, Simone Mori, William Nguyen, Bruno Conti, Benjamin F. Cravatt & Mario van der Stelt

Diacylglycerol lipases (DAGL) convert diacylglycerol to the endocannabinoid 2-arachidonoylglycerol. Our understanding of DAGL function has been hindered by a lack of chemical probes that can perturb these enzymes in vivo. Here, we report the design and synthesis of a set of centrally active DAGL inhibitors and activity-based probes and their use, in combination with chemical proteomics and lipidomics, to determine the impact of acute DAGL blockade on brain lipid networks in mice. Our findings using these novel chemical tools illuminate the highly interconnected and dynamic nature of lipid signaling pathways in the brain.

## Plenary lectures and focus sessions 7 December

### Focus session: Dynamics and kinetics of reactive and scattering processes

Chairs: Geert-Jan Kroes & Herma Cuppen

Research on bond cleavage and formation is central to chemistry. A wide range of experimental and computational techniques are applied, with some studies aiming for both high spatial and temporal resolution. In this focus session state-of-the-art research addressing the dynamics and kinetics of a wide range of reactive and scattering processes is presented.

Lectures:

1. Rainer Beck (EPFL, Switzerland)

*Exploring Gas/Surface Reaction Dynamics via Quantum State Resolved Molecular Beam Experiments*

We present recent results from our laboratory on quantum state resolved reactivity and state-to-state scattering measurements for the dissociative chemisorption of methane on Ni and Pt surfaces<sup>1-8</sup>. Methane dissociation plays an important role in the steam reforming process used to convert methane and water into a mixture of hydrogen and carbon monoxide by heterogeneous catalysis. Using state-selective reactant preparation by rapid adiabatic passage in a molecular beam, we prepare the surface incident methane and water molecules in specific ro-vibrational quantum states and measure the state-resolved reactivity on a single crystal surface using surface analytical techniques such as Auger electron spectroscopy, King & Wells beam reflectivity, and reflection absorption infrared spectroscopy (RAIRS). We also probe the quantum state distribution of the nonreactive scattered molecules by combining infrared laser tagging with bolometric detection. The results of our measurements provide evidence for mode- and bond-specificity as well as steric effects in chemisorption reactions and show that the dissociation of both methane and water cannot be described by statistical rate theory but require dynamical treatments including all internal vibrational and rotational degrees of freedom of the dissociating molecule. The detailed reactivity data obtained in our measurements serves as stringent test for the development of a predictive understanding of these industrially important gas/surface using first principles theory.

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2. D. Migliorini (LEI; Kroes)

*Accurate simulation of a polyatomic molecule-metal surface reaction: dissociative chemisorption of CHD<sub>3</sub> on Pt(111) and Ni(111)*

Davide Migliorini, Francesco Nattino, and Geert-Jan Kroes

Leiden Institute of Chemistry, Leiden University, Gorlaeus Laboratories, P.O. Box 9502, 2300 RA Leiden, The Netherlands

Although important to heterogeneous catalysis, until recently it has not been possible to model reactions of polyatomic molecules with metal surfaces with chemical accuracy. Partnering the specific reaction parameter

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(SRP) approach to density functional theory with Ab Initio Molecular Dynamics (AIMD) now enables this. This is demonstrated with AIMD calculations on CHD<sub>3</sub> + Ni(111) in which the SRP functional is fitted to supersonic beam experiments, and validated by showing that AIMD with the resulting functional reproduces initial-state selected sticking measurements with chemical accuracy (4.2 kJ/mol  $\approx$  1 kcal/mol). New results for CHD<sub>3</sub> + Pt(111) will be reported at the meeting.

3. A. Fredon (RU; Cuppen)

*Admolecules mobility on interstellar icy dust particles*

Ice covered dust grains play an important catalytic role in interstellar clouds. Gas phase species adsorb onto their surfaces, diffuse and react. Because of the low temperature, chemistry is limited to exothermic reactions and hence reaction products are excited. By performing thousands of Molecular Dynamics simulations, we investigate the fate of kinetically excited species; possible outcomes are diffusion over the surface, desorption, and distortion of the ice mantle. We consider a wide range of additional kinetic energy (0.5-5 eV) and different admolecule species (H<sub>2</sub>O, CH<sub>4</sub>, and CO<sub>2</sub>).

4. G. Shchygol (SCM; Goumans)

*Modeling reactions with ReaxFF in MOFs with defects*

Local and long-range defects strongly affect sorption and catalytic properties of metal organic frameworks (MOFs), but are very difficult to study both experimentally and computationally.

The reactive MD method ReaxFF is suitable to tackle such complex chemical systems, however, suitable force field parameters are usually not immediately available. We will discuss a systematic approach to tackle ReaxFF parameterization as well as automated tools for analyzing reactive events.

We improve the effectiveness of global optimization methods, which sample a vast, complex parameter space, by grouping ReaxFF parameters and statistically analyzing them across many sets, and applying smart filters.

## Plenary lectures and focus sessions 7 December

### Focus session: Bio-inspiration in chemistry

Chair: Bert Klein Gebbink

*"Bio-inspired Chemistry: Nature as a source of inspiration in chemistry"*

Like in the times Leonardo da Vinci was studying birds in his attempts to be able to fly, nature is an important source of inspiration for chemists. This session brings together a number of speakers from different chemical research fields with the aim to highlight the strength of bio-inspired approaches in chemistry. The speakers will detail their endeavours in the design and development of responsive polymeric materials (prof. Jan van Esch, TUD) and non-noble metal based catalysts through the use of concepts 'borrowed' from nature (dr. Pradip Ghosh, UU). In addition, Wilhelm Huck (RU) will explain how his group aims to mimic whole cells and study cellular processes through the use of nano-droplets.

Speakers:

#### 1. Wilhelm Huck (RU)

*The end of chemistry... the beginning of life*

Complex networks of chemical reactions together define how life works. We are familiar with the metabolic networks studied in biochemistry, and in recent decades many regularly recurring network motifs have been uncovered that are responsible for much of the functional behaviour in signalling or genetic networks. However, molecular 'circuits' are very delicate, and sensitive to changes in concentration, temperature, and so on. An important feature of self-organization in complex systems is that these systems can self-repair, even when perturbed significantly. In my lecture, I will show how we can explore the dynamic (i.e. robustness and resilience) of these reaction networks in response to global perturbations and follow the precise molecular trajectory during phase transitions.

#### 2. P. Ghosh (UU; Klein Gebbink)

*Proton and electron responsive  $\beta$ -diiminates: studies of redox activities in transition metal complexes*

The use of organic molecules as redox equivalents is of key importance in biological enzymatic transformations and Nature employs many different redox cofactors to promote long-range electron transfer reactions as part of such transformations. In addition, the redox chemistry of various enzymes is inherently proton-coupled, meaning that changes in electron inventory are accompanied by changes in proton content. For example, in small molecule models for tyrosinase phenol oxidation is reported to involve proton-transfer to an exogenous base and electron-transfer to an outer-sphere oxidant or electrode.

Here, we will introduce a new class of N,N-bidentate  $\beta$ -diiminate donor ligands, in which two 1-alkyl-4,5-disubstituted-1H-imidazole moieties are attached to a central methylene unit (HL = bis(1-methyl-4,5-diphenyl-1H-imidazol-2-yl)methane). These ligands are structurally very similar to  $\beta$ -diketiminates (NacNac-). In principle,  $\beta$ -ligand like HL can act as i) a neutral N,N donor ligand (HL), ii) a closed shell mono-anionic ligand (L<sup>-</sup>), and iii) a neutral n-radical ligand (L<sup>•</sup>). □). Herein, we report

complexes derived from HL, in which the ligand undergoes facile and reversible acid-base and redox chemistry. This has allowed us to characterize complexes with the ligand in the three different oxidation states. The corresponding zinc(II) complexes were synthesized as diamagnetic analogues, for which the Zn(II) center (d<sup>10</sup>, S = 0) is not expected to participate in redox chemistry and thus, the oxidation state of the ligand is expected to determine the overall charge of the complex. X-ray crystallography, electrochemistry, and various spectroscopic techniques in conjunction with Density functional theory (DFT) have been employed to elucidate the redox non-innocence character of the deprotonated ligand L<sup>-</sup> in these complexes.

#### 3. Jan van Esch (TUD)

## Plenary lectures and focus sessions 7 December

### Focus session: Self-organization at interfaces: from controllable interactions to 2D materials

Chair: Daniel Vanmaekelbergh

The assembly and anisotropic attachment of (nanocrystal) colloids at an interface constitutes a major route to novel nanostructured systems, which impact catalysis, logics and opto-electronics. The session will focus on the adsorption and interactions of nm to  $\mu\text{m}$  colloids at an interface, and the various nanostructured materials that have been prepared.

Speakers:

1. J.J. Geuchies (UU; Swart)

*Watching the birth of a nanocrystal Superlattice*

The formation of atomically coherent 2-D PbSe superstructures from nanocubic building blocks can result in long-range atomic and nanoscale order [1,2]. We have studied the mechanism of the formation of 2-D PbSe superstructures with square geometry using in-situ grazing-incidence x-ray scattering, ex-situ electron microscopy, and Monte Carlo simulations. The nanocrystals adsorb at the liquid-gas interface, followed by the formation of a hexagonal nanocrystal monolayer. As time progresses, the hexagonal layer is deformed to a square superlattice, due to the four-fold symmetry of the in-plane interaction caused by the PbSe nanocrystal facets. During these consecutive phase transitions the nanocrystals align themselves atomically and finally form atomic bonds.

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2. René van Roij (UU)

*Interfacial self-assembly of cubic nanocrystals*

3. Jasper van der Gucht (WUR)

*Self-organization by capillary interactions: the effect of interfacial curvature*

Particles adsorbed to a liquid interface with anisotropic curvature experience capillary interactions between them that are anisotropic. We present experiments and numerical calculations of the interaction potentials between the particles and show how these interactions give rise to organization into regular lattices.

4. Peter John Beltramo (ETH Zürich)

*Self-assembly at fluid-fluid interfaces*

Interfacial particle monolayers self-assemble due to variations in shape or topological heterogeneity that causes three phase contact line undulations that lead to lateral capillary interactions. The structures which result from this have exceptional mechanical properties and can be used to stabilize high interface systems and even arrest dissolution. In a first part of the talk I will discuss a strategy to arrest coalescence by interfacial rheology design. Nature's most ubiquitous self-assembled interface is the phospholipid bilayer, which comprises all cell and organelle membranes. In the second part of the talk, I will discuss a new technique to study such systems in a platform where the membrane interactions can be controlled and interrogated in a rational manner.

## Plenary lectures and focus sessions 7 December

### Focus session: Molecular organization and function of chromatin

Chair: Hugo van Ingen

Chromatin, the complex of DNA and its associated proteins, is crucial in the maintenance of genomic integrity and regulation of gene expression. Chromatin-binding proteins are emerging as a promising drug targets to combat disease. Using a molecular perspective, we present the challenges and opportunities in understanding chromatin function.

Speakers:

1. Sjaak Neefjes (LUMC)

*Identifying old anti-cancer drugs as new epigenetic modifiers: the anthracyclines*

Anthracyclines are effective and broadly used anti-cancer drugs. Their prime action is the inhibition of the enzyme topo-isomerase II resulting in DNA double stranded breaks. Tumor cells are supposedly more sensitive to DNA breaks which would explain the action of anthracyclines as cancer drugs. We have shown that these drugs also evict histones from chromatin, effectively altering the epigenome. We have identified variant drugs that only evict histones and still act as anti-cancer drugs, challenging the dogma of the action of these compounds. This separation of activities has major effects on the many side effects associated to these drugs including cardiotoxicity and second tumor formation. We are now preparing variant drugs for reintroduction in the clinic.

2. O. Ordu (TUD; Dekker)

*Investigating the handedness dynamics of tetrasomes*

The DNA of eukaryotic organisms is tightly packed into a hierarchical DNA-protein structure called chromatin in order to fit into the micron-scaled nucleus. Besides packaging DNA, chromatin also plays an essential role in genome regulation by controlling DNA accessibility. Its basic unit termed nucleosome consists of a short piece of DNA wrapped around a core of eight histone proteins. Nucleosomes assemble along a precise pathway in which tetramers of histones H3 and H4 bind to the DNA first, forming tetrasomes, and then two dimers of histones H2A and H2B complete the formation of full nucleosomes.

We investigate the assembly and structural dynamics of tetrasomes at single-molecule level by directly measuring the length and twist of individual DNA molecules using Freely-Orbiting Magnetic Tweezers (FOMT). By this means, we have studied both the replication-coupled histone H3.1 and its replication-independent variant histone H3.3. These tetrasomes have shown the remarkable feature of spontaneously changing their handedness between a preferentially occupied left-handed and a less populated right-handed state. Our current study on artificially modified tetrasomes lacking this handedness dynamics indicates that this feature results from thermal fluctuations at the H3-H3 interface. These findings reveal dynamic rearrangements of nucleosome structure to possibly regulate DNA-supercoiling.

3. Elzo de Wit (NKI)

*The cohesin release factor WAPL controls chromatin loop extension*

The spatial organization of chromosomes influences many nuclear processes ranging from DNA replication and repair to gene expression. My lab studies the 3D organization of the genome and the functional role this plays in regulating nuclear processes. To this end we use a combination of genomics methods such as ChIPseq, RNAseq and 3C-derived methods such as Hi-C and 4C. I will present recent results that provide insight into the role of the ring-shaped cohesin complex in organizing the 3D genome. Cohesin loops together convergent CTCF sites along chromosomes. We show with high-resolution Hi-C analysis that

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chromatin loop size can be increased, and that cohesin's DNA release factor WAPL restricts the degree of this extension. WAPL also prevents looping between incorrectly oriented CTCF sites. We find that WAPL deficiency bypasses the need for cohesin's DNA loader SCC4 and we reveal that SCC4 promotes the extension of chromatin loops. We provide functional evidence in support of the model that chromatin loops are processively enlarged by the extrusion of DNA from cohesin rings. We conclude that the balanced activity of SCC4 and WAPL enables cohesin to correctly structure chromosomes to ensure proper transcriptional control.

4. Abdenour Soufi (Univ. of Edinburgh)

### *Mechanistic Insights Into Cell Fate Conversion*

It is astounding to discover that it takes so few transcription factors (TFs) to convert cells from one type to another. Strikingly, the four TFs: Oct4, Sox2, Klf4, and c-Myc (OSKM) are able to convert fibroblasts to become induced pluripotent stem cells (iPSCs). To understand how OSKM initially target silent genes, we previously mapped the interaction of OSKM with the somatic genome early in reprogramming. We found that O, S, and K, but not Myc, engage closed chromatin at distal sites, a hallmark of pioneer activity. Here we investigate the differential interaction of O, S, K, and M with nucleosomes, both in vitro and in vivo. We reveal that the pioneer activity of reprogramming factors relates to the basic ability of TFs to adapt their DNA-binding domains (DBDs) to target partial motifs exposed on the surface of nucleosomes. Other DBDs that lack such adaptability can bind with pioneer factors to recognize degenerate motifs on nucleosomes. Together our data provide the molecular basis by which pioneer factors interact with nucleosomes to engage silent chromatin, endowing competence for subsequent gene activation.

## Plenary lectures and focus sessions 7 December

### Industry-meets-Science session: Molecular biosensors

Chair: Menno Prins

#### *Innovative technologies for point-of-care testing and body biomolecular monitoring*

Healthcare is developing toward highly personalized solutions, attuned to the needs of patients, based on real time, precise and reliable data. Important enablers are miniaturized and easy to use sensing devices, which help to improve the monitoring and treatment of patients. This includes devices for near-patient testing (point-of-care) as well as sensors that are worn on or in the body (in-vivo sensors). Therefore, in the coming decades biochemical sensing technologies are needed which are small, sensitive, accurate, easy to use, cost effective, and versatile. For this to become reality, novel sensing principles, molecular materials, and device concepts need to be investigated and developed.

Speakers:

1. Jack van den Eerenbeemd (Philips)

*The Effect of Reagents on the Performance of the Minicare I20 Point-of-Care System*

In immunoassays, reagents are added to improve performance characteristics such as sensitivity and robustness. The mode of impact of these reagents is often not well understood and, especially in integrated systems, can also be of a non-chemical nature. It will be demonstrated for the Philips Minicare I20 point of care system how unraveling the interactions between the assay and the optical detection system leads to insights that are relevant for assay developers.

2. Kristian Göeken (UT, Subramaniam)

*Localized surface plasmon biosensor*

Recent emergence of multiple drug resistant Tuberculosis has led to a need for point-of-care (POC) devices capable of sensitive on-site detection of early stage Tuberculosis. In this study, we report the development of a DNA/RNA sensor based on localized surface plasmon resonance coupling of nanoparticles. The sensor has the ability to detect sub-picomolar amounts of bacterial RNA in just a number of hours using equipment which can be feasibly scaled down to POC-applicable sizes. We will show results obtained with crude lysates of *M. Tuberculosis* and *S. Aureus* and present future strategies towards enhancing sensitivity.

3. Thomas Cremers (Brains On-Line)

*Enzyme-based in-vivo biosensing of neurotransmitters and metabolites*

4. Stefano Cappelli (TU/e, Prins)

*Biosensing based on particles and single-molecule methods for continuous monitoring*

Continuous biomolecular monitoring refers to the automatic and periodic measurement of biomolecules in or on the human body. The first major product in this field is the continuous glucose monitoring biosensor, which is based on the enzymatic conversion of glucose in skin. However, enzymatic sensing is not widely applicable for the detection of biomolecules such as proteins and drugs. To that aim, sensing principles are required based on molecular affinity binding rather than enzymatic conversion. In this presentation we will describe two affinity-based single-molecule techniques based on particles as well as prospects for integrating these methods into a biosensing system.



## Plenary lectures and focus sessions 7 December

### Industry-meets-Science session: Stimuli-Responsive Materials

Chair: Maarten Smulders

Drawing inspiration from Nature, chemists are becoming more and more adept at preparing materials that are sensitive to their environment and that can adapt their function to external influences. In this focus session, recent advances in creating such stimuli-responsive materials, as can be utilised in a range of applications, will be discussed.

Speakers:

1. Philip du Prez (Ghent University)

*Vitrimers: Recyclable Materials of the Future?*

'End-of-life' applications of fully cured resins remains an issue as these polymer networks cannot be reshaped, repaired or recycled. In this presentation, a new chemical class of crosslinked polymers, obtained from upscalable raw chemicals, will be reported. Although the formed chemical bonds are permanent ones, they can very rapidly exchange positions at higher temperatures. The reported patented material is a quite promising example of a recently discovered new class of polymers, coined 'vitrimers', a name that refers to their ability to be processed and recycled like glass.

2. Rolf van Benthem (DSM)

*Macromolecular architectures at DSM: polymer templated silication technologies for antireflective coatings*

Controlled nucleation and growth of silica nanoparticles at the interface of polymer dispersion particles is the cornerstone of DSM's technology for the fabrication of antireflective coatings for solar front cover glass panels (Same Sun, More Power TM). This presentation will highlight the scientific insights that enabled this controlled nucleation and, thus, opened the way to new opportunities for antireflective coating strategies.

3. Zeger Vroon (TNO)

*Window of the future (IR regulating windows)*

Windows play an important role in the energy use and balance of a building, as energy exchange through windows accounts for over 50% of energy consumed through a building's envelope by means of conduction, convection and radiation. However, since 1970 only two main developments have taken place in the window market: 1) the introduction of double/triple glass windows for improved insulation, 2) the introduction of low emissivity (low-e) coatings for improved energy control in the building. An ideal window for Western Europe will reflect IR light from the sun in the summer and transmit IR light in the winter. In the winter, the coated glass has to ensure that radiator heat from the building interior is reflected back into the building. Such so-called smart windows are able to perform optimally in summer and winter, e.g. through switching from an IR transmitting to an IR reflecting state at a specific temperature (thermochromic). In the coming 20 years a lot of new developments related to windows are needed. In his lecture Vroon will present the developments in IR regulating coating and energy generating windows.

## Plenary lectures and focus sessions 7 December

### Industry-meets-Science session: Continuous flow catalysis

Chair: Floris Rutjes

The majority of catalytic processes, in academia but also on larger scale in industry, are performed in conventional batch operations. During the past decade, however, microreactor technology has been developed allowing to routinely conduct chemical reactions in flow. The continuous mode of operation has intrinsic advantages with respect to safety, heat and mass exchange, control over reaction conditions and reproducibility. As a result, a strongly increasing number of (catalytic) reactions is currently being carried out in continuous flow, which in turn has also given a boost to developments in flow reactor technology. In this session, several of these aspects will be highlighted, both from fundamental and more applied points of view.

Speakers:

1. Jesus Alcazar (Janssen-Cilag)

*Flow Chemistry as a Tool for Drug Discovery*

Continuous flow chemistry has recently emerged as a novel chemical tool that can help synthetic chemists to combine efficiency and sustainability. The better efficiency of this technology over traditional batch approaches relies in its main advantages: High control of the reaction variables, such as reactants mixing, heat and mass transfer; access to novel process windows, reactions at high temperature and pressure; easier reproducibility and scalability, and increased surface to volume ratio. However, this technology did not attract much attention in Discovery, where speedy preparation of a pool of target compounds is usually required. Many Medicinal Chemists are still wondering what value Flow Chemistry adds over traditional batch parallel approaches and they foresee its potential application limited to resolving scaling up issues. In this presentation examples of applications of flow chemistry to Drug Discovery will be disclosed. This technology is currently having impact in all levels of the discover process, from Hit to Lead to Late Lead Optimization. Current status of implementation at Janssen and future directions will be also reported.

2. Hannes P. L. Gemoets (TU/e, Noël)

*CH-activation in continuous flow*

Recent development in the direct functionalization of carbon-hydrogen bonds changed the way chemists look at reactivity. C-H functionalization, a direct one-step synthetic strategy, has emerged as a powerful and efficient toolbox for carbon-carbon and carbon-heteroatom formation. However, the intrinsic low reactivity and high abundance of C-H bonds often hamper practical applications. In this work, continuous-flow chemistry has been employed as a novel tool to enable unprecedented transformations. Enhanced gas-liquid mass transfer, precise control of the residence time and efficient irradiation facilitated the C-H olefination<sup>1</sup>, arylation<sup>2, 3</sup> and acylation<sup>4</sup> of (hetero)arenes.

References:

1. H. P. L. Gemoets, V. Hessel and T. Noël, *Org. Lett.*, 2014, 16, 5800-5803.
2. H. Gemoets, I. Kalvet, A. Nyuchev, N. Erdmann, V. Hessel, F. Schoenebeck and T. Noel, *Chem. Sci.*, 2016, DOI: 10.1039/c6sc02595a.
3. N. Erdmann, Y. H. Su, B. Bosmans, V. Hessel and T. Noel, *Org. Process. Res. Dev.*, 2016, 20, 831-835.
4. U. K. Sharma, H. P. L. Gemoets, F. Schröder, T. Noël and E. V. Van der Eycken, (submitted), 2016.

3. Daniel Blanco Ania (RU, Rutjes)

*Expanding the Applications of Flow Chemistry: Heterogeneous Catalysis and Large-Scale Photochemistry*

Flow chemistry is a reasonably new technology whose rapid growth has been one of the most significant changes in the field of Organic Synthesis in recent times. Some flow processes were unresolved matters compared to the corresponding batch processes until recently (e.g., heterogeneous catalysis) and others

## Plenary lectures and focus sessions 7 December

have surpassed their batch counterparts (e.g., photochemistry). We present herewith two applications in these fields to contribute to the expansion of flow chemistry: 1) solid-supported copper-catalyzed pyrazole syntheses in continuous fashion with improved results over batch and 2) large-scale synthesis of (*E*)-cyclooctene derivatives in a continuous flow process.<sup>1</sup>

<sup>1</sup> J. Comas-Barceló, D. Blanco-Ania, S. A. M. W. van den Broek, P. J. Nieuwland, J. P. A. Harrity, F. P. J. T. Rutjes. *Catal. Sci. Technol.* **2016**, 6, 4718–4723.

<sup>1</sup> a) L. Maartense, D. Blanco-Ania, F. P. J. T. Rutjes, unpublished results. b) D. Blanco-Ania, S. A. Gawade, L. J. L. Zwinkels, L. Maartense, M. G. Bolster, J. C. J. Benninshof, F. P. J. T. Rutjes. *Org. Process Res. Dev.* **2016**, 20, 409–413.

## Plenary lectures and focus sessions 7 December

### Session organized by KNCV: Chemical entrepreneurship (startup and scale up)

Chair: Peter van Tilburg

Starting a new company involved in chemistry, biotechnology, Life sciences or materials requires a completely different approach (people, vision, financing, location, execution, time lines) and poses an enormous challenge. Based on own experiences we want to give you a flavor of the challenges to expect when becoming an entrepreneur.

Speakers:

1. Ton Vries (Syncom)

*Syncom, how changing markets bring new business opportunities*

Syncom has been active as a chemistry contract research organization (CRO) for almost 30 years serving the chemical and pharmaceutical R&D markets. The changes in especially the pharma R&D landscape have made a huge impact on the business models for R&D support.

In the last eight years Syncom has adapted its strategy via new collaborations, creating new business models, open innovation initiatives and setting up joint ventures.

The presentation will be about entrepreneurship in the CRO market and the many opportunities which the current market circumstances offer.

2. Marcel Oogink (Duplaco)

3. Tjeerd Barf (AstraZeneca)

*How (not) to start a biotech: From Dismissal to Deal*

In the year 2011, the majority of the pharma R&D activities of MSD in Oss were discontinued. Around 1,700 people were laid off, and the future for many had to be reshaped. Five years later, biotech and pharma are thriving again at Pivot Park. Acerta Pharma became operational early 2013, and was the subject of an acquisition only three years later. The amazing tale of this journey, as well as the personal experience of starting a biotech company will be shared.

4. Peter van Tilburg (Enzyep)

## Plenary lectures and focus sessions 7 December

### Session organized by KNCV: Chemistry Education in the Netherlands

Organized by the Commission Education and the Section Chemistry Education

Chair: Jeroen Cornelissen

Developments in Chemistry Education are at the heart of this session. Three presenters will guide us through their innovations: (1) excellence promoting educational materials, meant to enrich and deepen the pre-university (vwo) science content (2) innovative science education at lower secondary, (3) insights into the redesigned secondary vocational education (MBO).

Speakers:

#### 1. Excellence promoting educational materials

Ir. Geert H.F. Hurenkamp, K.S.G. De Breul Zeist/Rodenborch-College Rosmalen (*co-winner of the KNCV 2015 Chemistry Education Award*)

Examples of excellence promoting educational materials, primarily aimed at pre-university learners ('vwo', aged 16-18) are: a module in Nanoscience, material concerning electronic molecular structure and reactivity, and material in elementary (statistical) thermodynamics. Examples and the underlying 'principles' and requirements of these activities will be addressed.

#### 2. Create your own education!

Joris van Elferen, Mondial College Nijmegen (*co-winner of the KNCV 2015 Chemistry Education Award*)

Suppose you want a course book for physics and chemistry in junior high school that meets the following requirements: link up with year 10, having useful ICT, individually challenging and giving students options. In this presentation the presenter will explain why he choose to write his own course book.

#### 3. New curriculum MBO

Dr. Petra J.M. Bouten, Summa Laboratorium, Summa College, Eindhoven

In September this year a new curriculum in MBO chemical and biological analyst education will start for the first year students. The differences and similarities of old and new will be compared.

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## Keynotes and plenary speaker 7/8 December

### Keynotes:

Thursday 8 December 08:30 – 09:00 Auditorium

Jan van Hest: *Building life-like systems: artificial cells and organelles*

In nature many biological processes are compartmentalized to ensure their integrity and efficiency. Inspired by this phenomenon, we explore hybrid capsules based on a combination of proteins and amphiphilic block copolymers to construct bioactive compartments. In this lecture we will give a number of examples to highlight the versatility of this approach.

Intrinsically porous enzyme-loaded polymer vesicles, also known as polymersomes, have been explored as artificial organelles. We have been able to introduce these nanoreactors in living cells and have shown they can perform their function in this natural environment. We have furthermore investigated the encapsulation of multiple polymersome nanoreactors in a larger polymersome, to mimic the structural build-up of a eukaryotic cell. With this approach we were able to perform a multistep cascade reaction in a controlled fashion.

One important aspect of living systems is that they can communicate with and respond to changes in the environment. We have been able to build a synthetic cell in which an internal biocatalytic process was triggered by the external addition of small molecules. By adding different molecules, a different response was attained.

Living cells are able to move under the influence of outside chemical signals, a process known as chemotaxis. We have applied this concept to bowl-shaped indented vesicles, known as stomatocytes, in which enzymes can be effectively encapsulated. The enzymes were able to effectively convert fuel molecules into oxygen. Due to their anisotropic shape, this catalytic activity allowed the particles to move. By employing a chemical gradient chemotaxis in biological fluids with high level of efficiency was observed. We have furthermore been able to construct an enzyme network inspired by nature, which allows us to regulate the speed of the nanomotors via feedforward mechanisms, in a similar way as glycolysis functions in living cells.

Thursday 8 December 08:30 – 09:00 uur zaal 63/64

Peter Schoenmakers: *SEPARATION TECHNOLOGY FOR A MILLION PEAKS (STAMP)*

Mass spectrometry is a fantastic technique for chemical analysis and structure identification, but it cannot cope with the simultaneous introduction of many different analytes in vastly divergent concentrations. Therefore, the characterization of very complex samples requires extensive (pre-) separation. Conventional high-resolution liquid chromatography offers the capacity to separate up to about 1000 peaks in an overnight experiment (about 1 peak per minute). Comprehensive two-dimensional liquid chromatography (LC×LC) constitutes a great step forward. In the Dutch public-private project HYPERformance LC (NWO – TA-COAST) peak capacities of about 5,000 have been achieved within one hour (about 1 peak per second). Also, the analytical sensitivity (*i.e.* signal-to-noise ratio) has been greatly improved. Yet, even LC×LC does not suffice to address challenging problems, such as the characterization of the human proteome.

Spatial three-dimensional separations constitute a different approach. The components in a sample are separated by migrating them to different positions in a three-dimensional separation body, first in one dimension and then in another, perpendicular one. The spatially separated sample is subsequently eluted in a third dimension and prints of the separated sample are obtained at regular intervals. Imaging methods can be used to analyse each “STAMP” of the effluent. If such a process can be realized in practice a dramatic increase in separation power is predicted. Up to a million peaks may theoretically be separated in an overnight run. The STAMP project is conducted with support from the European Union (ERC Advanced Grant).

## Keynotes and plenary speaker 7/8 December

Thursday 8 December 08:30 – 09:00 uur zaal 82/83

Tjeerd Barf: *Covalent Kinase Inhibition as A Versatile Approach in Drug Discovery*

Numerous covalent binding drugs have successfully entered the market and benefit patients with a variety of disorders. The general concept of covalent inhibition can be widely applied to the majority of the protein target families, and is no longer limited to enzyme families with catalytically active amino acid residues. Selective targeting of specific non-catalytically active cysteines in the ATP pocket of kinase has resulted in the identification of potent and selective kinase inhibitors with a beneficial pharmacodynamic profile.

This class of kinase inhibitors can offer distinct advantages in terms of potency, selectivity and prolonged in vivo efficacy, since the duration of action becomes a function of target protein turnover, rather than the pharmacokinetics profile of the inhibitor. Irreversible kinase inhibitors behave in a non-ATP competitive manner, which is a major upside in our collective efforts to master the human kinome. Typically, high intracellular ATP levels render conventional reversible kinase inhibitors less efficacious in a cellular context. This drop in potency is generally not observed when comparing biochemical and cellular assay data obtained with irreversible kinase inhibitors. Although potential liabilities such as toxic events have to be considered when embarking on the covalent binding principle, appropriate toolbox assays may help to screen for the most promising candidates with a good therapeutic window.

A few years ago, afatinib was approved by the US Food and Drug Administration (FDA) as the first covalent and irreversible binding kinase inhibitor. Afatinib blocks the epidermal growth factor receptor (EGFR) and shows efficacy in patients with metastatic lung cancer (NSCLC). Around the same time frame ibrutinib, an irreversible inhibitor of Bruton Tyrosine Kinase (BTK), obtained breakthrough registration in different B cell lymphoma subtypes. Several other irreversible kinase inhibitors – including Acerta's BTK inhibitor acalabrutinib – are currently undergoing clinical trials

## Keynotes and plenary speaker 7/8 December

Thursday 8 December 15:45 – 16:15 zaal 63/64

Thorsten Bach: *Chirality and Light: Enantioselective Catalysis of Photochemical Reactions*

[2+2] Photocycloaddition reactions belong undisputedly to the most important reaction classes in photochemistry. The creation of up to four new stereogenic centers in a single step and the further use of the formed cyclobutane rings – either directly or after appropriate ring opening – are hallmarks of this powerful transformation. In our group, we have studied two different approaches to achieve a catalytic enantioselective reaction course in [2+2] photocycloaddition reactions. The first approach is based on a triplet energy transfer by hydrogen-bonding chiral catalysts, which in turn are derived from a previously described template successfully employed in the total synthesis of (+)-meloscine. The second approach relies on chiral Lewis acids, which change the photophysical parameters of the substrate and allow a selective excitation in the chiral environment, which they provide.

A chiral xanthone turned out to be an efficient organocatalyst providing good turnover (10 mol%) and high enantioselectivities (>90% ee) in [2+2] photocycloaddition reactions while a related chiral thioxanthone allowed for enantioselective reactions promoted by visible light. Apart from this approach, we have also looked into the possibility of Lewis-acid mediated enantioselectivity in photochemical reactions. Chiral Lewis acids were developed for [2+2] photocycloaddition reactions and are currently being further explored.

The presentation discusses the background of the above-mentioned studies and provides the latest results of our research efforts in this area.

Thursday 8 December 15:45 – 16:15 zaal 82/83

Carsten Schultz: *Tools for imaging and manipulating cellular networks*

Our group is interested in developing tools but also in applying these in the discovery of new functional aspects of signaling networks in intact cells. We focus largely on signaling networks governing immediate physiological responses such as receptor internalization and secretion. I will present small molecule tools such as caged or photoswitchable molecules and chemical dimerizers to specifically elevate the concentration of a signaling molecule. These tools are applied in model cells that express fluorescently tagged molecules to detect changes in the signaling network of  $\beta$ -cells including the first ratiometric reporter to monitor insulin secretion of beta-cells in realtime. I will also show how changes in the lipid composition alters the structure and function of the secretory vesicles as is detected by correlative fluorescence and electron microscopy (CLEM). Time permitting I will disclose a new cellular function of sphingosine found by using a caged version of the lipid.

Thursday 8 December 15:45 – 16:15 Auditorium

David Leys: *Serendipitous discovery of enzymatic 1,3 dipolar cycloaddition: nature can put 2 and 3 together*

In contrast to the organic chemist, Nature appears to have rarely made use of pericyclic reactions. By investigating the mechanism of the UbiX-UbiD enzyme system, we uncovered data that suggests Nature does use 1,3 dipolar cycloaddition. The UbiX-UbiD system has been shown to interconvert unsaturated hydrocarbons (often aromatic) with corresponding  $\alpha$ - $\beta$  unsaturated carboxylic acids (i.e. the dipolarophile). Our recent work on these enzymes demonstrates UbiD acts as the (de)carboxylase and relies on a novel cofactor: a prenylated flavin (prFMN). The latter is made by UbiX in the reduced form, and oxidative maturation of the cofactor is proposed to take place within the UbiD active site. The maturation generates an iminium form of the cofactor (prFMN-iminium) that has azomethine ylide character (i.e. the dipole). We propose a transient 1,3-dipolar



## Keynotes and plenary speaker 7/8 December

cycloaddition between cofactor and the alkene substrate underpins the reversible decarboxylation step. New data completing the UbiX-UbiD mechanistic picture will be presented.

### References:

- Sweating the assets of flavin cofactors: new insight of chemical versatility from knowledge of structure and mechanism, D Leys, NS Scrutton (2016), *Current opinion in structural biology* 41, 19-26
- Biochemistry: Unexpected role for vitamin B2, CF Clarke, CM Allan (2015), *Nature* 522, 427–428
- Natural 1,3-Dipolar Cycloadditions, M Baunach, C Hertweck (2015), *Angewandte Chemie International Edition*, 54, 12550
- New cofactor supports alfa-beta-unsaturated acid decarboxylation via 1, 3-dipolar cycloaddition, KAP Payne, et al. (2015), *Nature* 522, 497-501
- UbiX is a flavin prenyltransferase required for bacterial ubiquinone biosynthesis, MD White, et al. (2015), *Nature* 522, 502-506

**Plenary lecture:** 16:20 – 17:05 Benelux zaal

Georg Seelig: *Dynamic DNA nanotechnology from the test tube to the cell*

The programmability of Watson–Crick base pairing, combined with a decrease in the cost of synthesis, has made DNA a widely used material for the assembly of molecular structures and dynamic molecular devices. Working in cell-free settings, researchers in DNA nanotechnology have been able to scale up system complexity and quantitatively characterize reaction mechanisms to an extent that is infeasible for engineered gene circuits or other cell-based technologies. However, the most intriguing applications of DNA nanotechnology — applications that best take advantage of the small size, biocompatibility and programmability of DNA-based systems — lie at the interface with biology. Here, we review recent progress from our lab in the transition of dynamic DNA nanotechnology from the test tube to the cell.

## Abstracts parallel speakers 7/8 December

### Room 55-57: Analytical Tools I

7th December 2016, 19.25 – 19.45

#### *Overhauser Dynamic Nuclear Polarization for high sensitivity NMR in supercritical CO<sub>2</sub>*

Bas van Meerten (RU), Michael Tayler, Arno Kentgens and Jan van Benthum

Overhauser Dynamic Nuclear Polarization (ODNP) is a well known technique to improve NMR sensitivity in the liquid state, where the large polarization of an electron spin is transferred to a nucleus of interest by cross-relaxation. The efficiency of the Overhauser mechanism for dipolar interactions depends critically on fast local translational dynamics at the timescale of the inverse electron Larmor frequency. The maximum polarization enhancement that can be achieved for <sup>1</sup>H at high magnetic fields benefits from a low viscosity solvent. In this contribution we investigate the option to use supercritical CO<sub>2</sub> as a solvent for Overhauser DNP. We have investigated the diffusion constants and longitudinal nuclear relaxation rates of toluene in high pressure CO<sub>2</sub>.

The change in <sup>1</sup>H T<sub>1</sub> by addition of TEMPO radical was analyzed to determine the Overhauser cross-relaxation in such a mixture, and is compared with calculations based on the Force Free Hard Sphere (FFHS) model. By analyzing the relaxation data within this model we find translational correlation times in the range of 2-4 ps, depending on temperature, pressure and toluene concentration.

7th December 2016, 19.45 – 20.05

#### *Making Analytically Incompatible Approaches Compatible*

Bob Pirok (UVA), Fleur van Beek, Wim Genuit, Ron Peters

The project MANIAC (Making Analytically Incompatible Approaches Compatible) provides a generic approach for coupling two vast "orthogonal" domains, i.e. chemistry (chemical reactions and processes) and physics (modern methods of instrumental analysis). The MANIACal strategy is based on the use of (physical) modulators (MO) and chemical modulation reactors (MORE).

For example, the MANIAC approach is used to characterize nanoparticles, degrade them, and then characterize the constituting molecules using chromatographic, mass-spectrometric or spectroscopic methods. Likewise, natural polymers (cellulose, hemicellulose, lignin) and microbial reactions can be studied. In all cases automated MANIAC measurements yield more information in a much shorter time.

## Abstracts parallel speakers 7/8 December

### Room 58: Mechanism of chemical reactions

7th December 2016, 19.25 – 19.45

#### *Bite-angle bending as key for understanding metal reactivity of d10-[M(NHC)2] complexes*

Jörn Nitsch (VU), Florian Hering, Ursula Paul, Lando P. Wolters, Célia Fonseca Guerra, Andreas Steffen, Udo Radius, F. Matthias Bickelhaupt

d10-Transition metal complexes bearing phosphine or NHC ligands play a vital role in catalysis. We note that 14, 16 and 18 VE d10 transition metal PPh<sub>3</sub> complexes are well known, but higher coordination numbers > 2 of homoleptic d10 NHC complexes are very rare, and 18 VE [M(NHC)<sub>4</sub>] compounds are completely unknown. We determined the factors which are important for the stability of higher coordinated [M(NHC)<sub>4</sub>] species. The scope of our findings can be extended beyond the present NHC model systems and has wider implications the reactivity of group 10 NHC complexes.

7th December 2016, 19.45 – 20.05

#### *Fluorescent cinchona alkaloids for single molecule studies of organocatalysis*

Dongdong Zheng (UvA), Mina Raeisolsadati Oskouei, Dina Petrova, Hans Sanders, Fred Brouwer

Single-molecule fluorescence due to its potential to detect rare events has proven useful for the investigation of catalytic reactions, e.g. with enzymes and zeolites. Applications in molecular chemistry are still rare. We report a fluorescently labelled cinchona alkaloid that acts as asymmetric organocatalyst for a number of reactions. In polar solvents, the fluorescence of the compound is quenched by electron transfer, but this process is suppressed when the catalyst binds to a substrate. We will briefly present the photophysical behavior and show experiments aimed at a direct observation of catalytic events in a simple organic reaction.

## Abstracts parallel speakers 7/8 December

### Boszaal: Multicomponent reactions

7th December 2016, 19.25 – 19.45

#### *Stereoselective one-step synthesis of complex alkaloid mimics by an interrupted Ugi cascade reaction*

Jordy M. Saya (VU), Barry Oppelaar, Romano V.A. Orru, Eelco Ruijter

Tryptamine-derivatives isocyanides react with various aldehydes and amines in an interrupted Ugi cascade reaction to form complex tetracyclic heterocycles reminiscent of bioactive alkaloids. The reaction proceeds with complete diastereoselectivity at ambient temperature in the absence of any catalyst or other reagents. The products can undergo a variety of complexity-generating secondary transformations to provide access to a diverse array of medicinally relevant small molecules in a highly efficient sequence.

7th December 2016, 19.45 – 20.05

#### *Exploiting isocyanide-based multicomponent reactions in the design of small-molecule libraries*

Veronica Estevez Closas (VU), Eelco Ruijter, Romano V.A. Orru

The European Lead Factory (ELF), a pan-European platform, was set to give a major boost to drug research in Europe, comprising a collection of half a million compounds and a screening centre. Our contribution to this consortium consists of the design of new libraries of compounds exploiting the potential of multicomponent reactions (MCRs) as highly convergent and diversity-generating processes. Specifically, we have exploited recently some isocyanide-based multicomponent reactions (IMCRs) in combination with complexity-generating reactions to prepare new nitrogen-rich scaffolds. These strategies provide straightforward access, from commercially available starting materials, to small molecules with drug-like molecular properties, novelty and diversity potential among their features.

## Abstracts parallel speakers 7/8 December

### Room 63/64: Backer lecture

7th December 2016, 19.25 – 20.05

*Advancing selectivity control with highly reactive organometallic reagents*

Masimo Giannerini (*Janssen Pharmaceuticals, Inc.*)

The high reactivity of Grignard and organolithium reagents has been recognized since the early stages of synthetic organic chemistry as an invaluable tool to induce fast and effective C-C bond formation. Dealing with such an outstanding reactivity, selectivity issues may easily arise when different reaction modes are available for these organometallics. Despite the efforts devoted in developing increasingly daring and selective reactions involving reactive organometallics, still many challenges and opportunities lie ahead of us. Cu-catalyzed asymmetric allylic alkylations (AAA) and Pd-catalyzed cross-couplings (CC) represent the ideal playground to unveil unprecedented level of selectivity control and to unleash the synthetic potential of this class of reagents.

Cu-catalyzed AAA with reactive organometallic reagents require fine selectivity control, dealing with regio-chemo- and enantioselectivity at once. The discovery of an AAA with Grignard reagents proceeding also with exquisite Z-selectivity is presented as well as the total reverse of regioselectivity in allylic alkylations with organolithium compounds dictated exclusively by the ligand choice.

Pd-catalyzed CC between organo(pseudo)halides and organometallic compounds are indispensable tools in modern organic chemistry. Once selectivity issues are brought under control, the strong reactivity of organolithium compounds can be deployed performing highly demanding couplings, even in the absence of any additional solvent, within short reaction times (down to minutes) and under mild conditions.

## Abstracts parallel speakers 7/8 December

### Parkzaal: Applied microbial mechanisms

7th December 2016, 19.25 – 19.45

#### *Syngas fermentation by synthetic co-cultures of anaerobic microorganisms*

Diana Z. Sousa (WUR), Martijn Diender, Alfons J.M. Stams

Microbial syngas fermentation is an alternative way to convert biomass to valuable products. We study microbial co-cultures to produce target compounds. *Clostridium autoethanogenum*, a carboxydophilic acetogen, was co-cultured with *Clostridium kluyveri*, a bacterium employing the reverse  $\beta$ -oxidation pathway. *C. autoethanogenum* uses the syngas to produce acetate and ethanol, which are subsequently used by *C. kluyveri* to produce butyrate and caproate. Interestingly, *C. autoethanogenum* is able to convert these acids to butanol and hexanol, respectively. Currently we investigate how environmental factors influence production patterns. Genome-based modelling is applied to steer the production to only acids or only alcohols.

7th December 2016, 19.45 – 20.05

#### *Assessing diol dehydratase from *Lactobacillus brevis* for 2-butanone production*

Rosario Medici (TUD), Linda G. Otten, Ulf Hanefeld

2-butanone (MEK) is an industrial solvent and building block. Its major drawback is that it is produced by non-sustainable methods, relying on fossil fuels. Here, we describe a biobased route. Starting from sugars, we use a sequence of enzymes to produce MEK. Results for the key step, the dehydration meso-2,3-butanediol catalyzed by diol dehydratase, will be presented. The corresponding genes from *Lactobacillus brevis* were cloned and recombinantly expressed in *E. coli*. This strain produces MEK yielding 0.24 g L<sup>-1</sup> in 2 days. Strategies implemented to improve productivity, such as co-expression with meso-2,3-butanediol synthetic pathway or coenzyme regeneration, will be discussed.

## Abstracts parallel speakers 7/8 December

### Auditorium: Fluorescent sensors and imaging

7th December 2016, 19.25 – 19.45

#### *Novel fluorescent proteins applied in multiplexing of FRET sensors*

Marieke Mastop (UvA), Theodorus W.J. Gadella jr., Joachim Goedhart

Genetically encoded biosensors based on fluorescent proteins (FPs) enable the study of intracellular signaling processes in single living cells. Signaling outcomes are, however, often the result of multiple events. Therefore, multiplex functional imaging is necessary to understand signaling networks. A special class of FPs with a large difference between excitation and emission maximum (large Stokes shift or LSS) seem particularly suited for imaging multiple events. We have evaluated existing LSS FPs and engineered improved variants. We demonstrate that new sensors based on improved LSS FPs allow multiplex functional imaging of intracellular signaling.

7th December 2016, 19.45 – 20.05

#### *Engineering bioluminescent sensor proteins for smartphone-based antibody diagnostics*

Remco Arts (TU/e), Benice C.B. van Gerven, Marina D.B. Sabbadini, Susann K.J. Ludwig, Martijn van Rosmalen, Ilona den Hartog, Stefan Zijlema, Vito Thijssen, Stan van der Beelen, Maarten Merkx

Antibody detection is of fundamental importance in many diagnostic assays, yet current detection techniques tend to be cumbersome and/or expensive. We developed a new sensor platform (LUMABS) based on Bioluminescence Resonance Energy Transfer that allows antibody detection using a smartphone as the sole piece of equipment. The bright and stable emission of LUMABS changes from green to blue upon antibody binding, allowing the detection of pM concentrations directly in blood plasma. The modular sensor architecture can be generally applied for detection of any antibody and should also allow expansion of our approach to other biomarkers and therapeutic drug monitoring.

## Abstracts parallel speakers 7/8 December

### Room 82/83: NMR methods

7th December 2016, 19.25 – 19.45

*Protein assignment using paramagnetic effects with PARAssign*  
Mathilde Lescanne (LEI),

The liquid state NMR spectrum assignment of a protein is the first step of any further NMR study. It remains challenging for big proteins, and sometimes impossible with classical NMR assignment approaches. Using pseudocontact shifts (PCS) induced by several paramagnetic probes and the structure of the protein, PARAssign software assigns protein spectrum requiring datasets from simple 2D-HSQC NMR experiments. We demonstrate here the ability of PARAssign to assign with experimental PCS datasets the NMR methyl groups spectrum of the N-terminal domain of Hsp90 (25KDa).

7th December 2016, 19.45 – 20.05

*Novel high-sensitivity approaches for in-situ NMR*

D. Mance (UU), S. Narasimhan R. Damman, C. Pinto, M Daniels, G. Folkers, K. Houben, M. Weingarth, M. Baldus

NMR provides increasing opportunities to probe molecular structure and dynamics in intact molecular systems. High sensitivity and resolution is a critical requirement for such studies [1-3]. In our contribution, we report on the latest developments to design hyperpolarization methods and tailored proton-detection techniques for this purpose. We outline the chemical design principles and spectroscopic implementation. Applications ranging from the study of intact cell preparations to the analysis of (bio)materials will be shown.

[1] D. Mance et al., ACIE (2015) 54, 1579

[2] M. Kaplan et al., Nature Methods (2015) 12, 649

[3] A. Jantschke, Koers et al., ACIE (2015) 54, 15069



## Abstracts parallel speakers 7/8 December

### Room 80/81: (Prote)omics

7th December 2016, 19.25 – 19.45

#### *A proteomic approach for identifying new key components of the chemotaxis signaling pathway*

Marion Kamp (RUG), Arjan Kortholt and Peter J.M. van Haastert

Chemotaxis, or directional movement towards extracellular chemical gradients, is necessary for processes as diverse as finding nutrients, wound healing and metastasis. Previously, we have identified a basal signaling module that is essential to induce chemotaxis in the model organism *Dictyostelium*. Here we have used an extensive and efficient proteomic approach to identify further components of this basal signaling pathway that collectively form the dynamic signaling network for chemotaxis. The biochemical characterization of this network, which consists of a few hundred proteins, will help to understand the complex chemistry that cells use for adaptation in dynamic environments.

7th December 2016, 19.45 – 20.05

#### *Quantitative Mass Spectrometry to identify targets of Peroxiredoxin dependent Redox Signaling*

Loes van Dam (UMCU),

Redox signaling is a vital cellular process that proceeds through oxidative modification of cysteines. Paradoxically, the cysteines in many proteins that have been reported to be subject to redox signaling are poorly reactive with  $H_2O_2$  as compared to the active-site cysteines in the highly abundant 2-Cys peroxiredoxins. We hypothesized that oxidized peroxiredoxins can act to oxidize cysteines in specific targets. We used a mass spectrometry-based approach to identify oxidation-dependent interactions of each of the five 2-Cys peroxiredoxins. We propose that each peroxiredoxin acts as  $H_2O_2$  receptor to oxidize a specific subset of targets in redox signaling.

## Abstracts parallel speakers 7/8 December

### Room 65: Transcriptional regulation

7th December 2016, 19.25 – 19.45

*Ezh2 is not essential for early embryonic development but is required for tissue maintenance in zebrafish*

Julien Rougeot (RUMC)

Enhancer of zeste homolog 2 (Ezh2) is a Polycomb group protein that places the transcriptional repressive H3K27me3 mark and is important for embryonic development. We generated maternal zygotic *ezh2* mutant zebrafish embryos, which complete gastrulation and die during organogenesis (2 dpf), displaying pleiotropic phenotypes. However, gene expression analysis indicated that Ezh2 regulates maternal mRNA loading of zygotes and has a minor regulatory role during early zygotic gene expression (1 dpf). At this time, repressive epigenetic marks are lost whereas the activating mark H3K4me3 is globally not changed in the mutant. These results suggest a buffering mechanism between maternal mRNA load, zygotic expression and epigenetic control of transcription to ensure effective early embryonic development.

7th December 2016, 19.45 – 20.05

*Using CRISPR/Cas9 to unravel the role of mammalian RNAi in antiviral immunity*

Susan Schuster (RUMC), Lotte Tholen, Ronald P. van Rij

The RNA interference pathway (RNAi) is conserved amongst invertebrates and vertebrates and is crucial for antiviral immunity in plants, fungi and invertebrates. Recent evidence also suggests an antiviral role for RNAi in mammals, particularly in embryonic stem cells. In our study, we investigated whether RNAi contributes to antiviral immunity in differentiated cells. Our findings suggest that Ago2 deficient HeLa cells have higher viral loads and are stronger inducers of ISGs in response to poly (I:C) and positive sense RNA virus infection. Our results suggest that RNAi may have an immune modulatory role in response to viral challenge.

## Abstracts parallel speakers 7/8 December

### Room 55-57: Hyphenated MS Analysis

8th December 2016, 09.05 – 09.25

*In-depth Site-Specific N- and O-Glycosylation Analysis of Human C1-Inhibitor by C18-PGC-LC-MS/MS*  
Kathrin Stavenhagen (LUMC), Manfred Wuhrer

8th December 2016, 09.25 – 09.45

*Nanofractionation analytics with parallel mass spectrometry for identification of cytochrome P4501A2 inhibitors in metabolic mixtures*

Barbara M. Ziętek (VU), Marija Mladić, Ben Bruyneel, Wilfried M. A. Niessen, Govert W. Somsen, Jeroen Kool

This research focuses on the development and optimisation of an at-line nanofractionation methodology with parallel mass spectrometry (MS) for the detection and identification of CYP1A2 inhibitors present in metabolic mixtures. The platform is composed of a high performance liquid chromatography separation via a split coupled to high resolution nanofractionation and to MS. Six second fractions of eluate are collected on a 384-well microtiter plate, freeze-dried, and exposed to a fluorescence-based bioassay. A negative peak in the reconstructed bioactivity chromatogram is observed when metabolites inhibiting the CYP1A2 enzyme are present in the sample.

8th December 2016, 09.45 – 10.05

*Probing protein heterogeneity, conformation and affinity by combining native capillary electrophoresis with MS and SPR*

Elena Dominguez-Vega (VU), Anne-Lise Marie, Laura Bertoletti, Rob Haselberg, Jeroen Kool, Gerhardus J. de Jong, Govert W. Somsen

Assessment of the conformation and binding of individual components of protein mixtures requires separation techniques that preserve native macromolecular structures. Capillary electrophoresis (CE) provides proteoform resolution under near-physiological conditions, while maintaining protein affinity and conformational integrity. We present the combination of native CE with mass spectrometry (MS) and surface plasmon resonance (SPR) as new tools for the determination of conformers and affinity of proteins in complex samples. These systems permit assignment of unfolding intermediates and conformers of amyloidogenic and pharmaceutical proteins, as well as assessment of inhibitor and antigen affinities to heterogeneous enzymes and antibodies.

### Boszaal: Supramolecular Chemistry I

8th December 2016, 09.05 – 09.25

*Multiply hydrogen-bonded arrays from a quantum chemical perspective*  
Stephanie van der Lubbe (VU), Francesco Zaccaria, Célia Fonseca Guerra

## Abstracts parallel speakers 7/8 December

Hydrogen bonds play a crucial role in biochemical processes and many applicative fields of supramolecular chemistry. The strength of hydrogen bonds is still rationalized with textbook knowledge derived from experimental findings. We show that with state-of-the-art quantum chemical computations a profound understanding of the hydrogen bonding mechanism can be obtained for multiply hydrogen-bonded arrays. Hitherto unknown factors, which govern the strength of the hydrogen bonds, will be presented and discussed.

8th December 2016, 09.25 – 09.45

### *Orthogonal Functionalization of Ferritin via Supramolecular Re-Assembly*

Silvia J. Spa (LUMC), Anton Bunschoten, Marcus T.M. Rood, Ruud J.B. Peters, Abraham J. Koster, Fijs, W.B. van Leeuwen

In nature, supramolecular protein assemblies provide functional structures such as bio-nanoparticles. Ideally, such particles can controllably be tailored with multiple functionalities. To investigate if the degree of ferritin functionalization could be controlled using the self-assembly process, two photophysically distinct Cy3- or Cy5- functionalized ferritin batches were created. After dis-assembly, Cy3-, Cy5- and non-functionalized subunits were mixed in variable ratios. Photophysical measurements revealed the mixing-ratio was indicative for the ratios of subunits in the re-assembled capsids. The biomineralization properties of ferritin were retained in the multi-functionalized capsids. Combined, these data indicate that ferritin can orthogonally be functionalized using the self-assembly process.

8th December 2016, 09.45 – 10.05

### *Towards Self-Replicating Molecules Forming Compartments*

Boris Bartolec (RUG), Sijbren Otto

Spontaneous emergence of entities capable of self-replication combined with formation of compartments brings together two important aspects of life de novo as well as origin of life research. We designed an amphiphilic building block that can form a library of different interconverting oligomers through a dynamic combinatorial chemistry approach. Diverse bilayer assemblies are formed by selective incorporation of oligomers with specific structures. This process, coupled with potentially auto-catalytic growth, provides a unique example of a self-assembled chemical system that captures various aspects observed in cellular life.

## Abstracts parallel speakers 7/8 December

### Room 63/64: Chemistry controlled with light

8th December 2016, 09.05 – 09.25

#### *Muscle-like responses in light-driven polymer springs*

F. Lancia (UT), A.-D. Nguindjel, S.-J. Asshoff, N. Katsonis

We have demonstrated that the light-induced motion of a molecular switch can be amplified in liquid crystal polymer springs by using a strategy inspired from the biological world, and therefore can be used to produce work (Nature Chemistry, 2014). Here we evidence that these biomimetic springs show a non-linear elastic behavior that is comparable to the mechanical properties of muscle fibers (Nature Protocols, 2016). The springs also display strain-stiffening properties that can be controlled by photo-activation of the molecular switch. The mechanical properties of these molecular materials pave the way towards new applications for human-friendly and soft robotics.

8th December 2016, 09.25 – 09.45

#### *Rapid surface functionalization of hydrogen-terminated silicon by alkyl silanols*

Jorge Escorihuela (WUR), Han Zuilhof

Surface functionalization of inorganic semiconductor substrates, particularly silicon, has focused attention towards many technologically important applications, involving photovoltaic energy, biosensing and catalysis. For such modification processes, oxide-free (H-terminated) silicon surfaces are highly required and different chemical approaches have been described. However, their reactivity is often poor, requiring long reaction times (2-18 h) or the use of UV light (30 min). Here, we report a simple and rapid surface functionalization for H-terminated Si(111) surfaces using alkyl silanols.

8th December 2016, 09.45 – 10.05

#### *Developing a bacterial semi-organelle into photo-responsive protein systems*

Rindia M. Putri, J. Wilfried Fredy, Melissa S.T. Koay, Jeroen J.L.M. Cornelissen and Nathalie Katsonis

## Abstracts parallel speakers 7/8 December

### Room 58: Anticancer drug approaches

8th December 2016, 09.05 – 09.25

*D- versus L-glucose: Mitochondrial targeting of a light-activated dual-mode of action ruthenium-based anticancer prodrug*

Lucien Lameijer, Samantha Hopkins, Tobias Brevé, Sven Askes, Sylvestre Bonnet

Light-activated ruthenium anticancer prodrugs often suffer from poor water solubility, poor selectivity, and/or ill-defined intracellular targets. Two enantiomers of a glycoconjugated ruthenium drug were synthesized to allow direct comparison of the effect of chirality of the glucose moiety on uptake, toxicity, and localization of the prodrug without changing its physico-chemical properties. Both compounds showed different cytotoxicity in lung- and breast cancer cells in the dark, whereas similar ( $<1\ \mu\text{M}$ ) cytotoxicities were observed following low doses of visible light irradiation. Irrespective of chirality the emissive ruthenium complexes were found in the mitochondria, where two modes of action may contribute to light-induced cell death.

8th December 2016, 09.25 – 09.45

*Understanding the Mechanisms of Action of the Synthetic Bleomycin Mimic N4Py in Human Cell Cultures*

Arjan Geersing (RUG), Monique van der Wijst, Marianne Rots and Gerard Roelfes

Even after many years of research, little is known about the mechanism of action of the anti-tumor drug Bleomycin and its synthetic mimic N4Py. Here we will show that the function of different N4Py-fluorophore conjugates in live cells seem to deviate significantly from each other and, most importantly, from N4Py. This work will reveal that fluorophores can significantly change the biological activity of N4Py regarding cell uptake mechanisms, cellular localization and cell death mechanisms.

8th December 2016, 09.45 – 10.05

*Potent Inhibitors of Protein arginine N-methyltransferase designed to occupy both substrate binding sites*

Matthijs van Haren (UU), Linda Quarles van Ufford, Ed E. Moret, and Nathaniel I. Martin

The protein arginine N-methyltransferases (PRMTs) are a family of enzymes that function by specifically transferring a methyl group from the cofactor S-adenosyl-L-methionine (AdoMet) to the guanidine group of arginine residues in target proteins. Most notable is the PRMT-mediated methylation of arginine residues that are present in histone proteins which can lead to chromatin remodelling and influence gene transcription. A growing body of evidence now implicates dysregulated PRMT activity in a number of diseases including various forms of cancer. The development of PRMT inhibitors may therefore hold potential as a means of developing new therapeutics. We here report the synthesis and evaluation of a series of small molecule PRMT inhibitors designed to simultaneously occupy the binding sites of both the guanidino substrate and AdoMet cofactor. Potent inhibition ( $\text{IC}_{50}$  values in the nanomolar range) and surprising selectivity was observed when testing these compounds against a panel of methyltransferases.

## Abstracts parallel speakers 7/8 December

### Parkzaal: Photochemistry and photoresponsive molecules

8th December 2016, 09.05 – 09.25

#### *A 'Combinatorial Explosion' of Products through Photo-Chemo-Enzymatic Cascades*

W. Zhang (TUD), L. Leemans Martin, E. Fernandez Fueyo, M. Pesic, R. Wardenga, W. Kroutil, S. Schmidt, F. Hollmann

Currently, the combination of chemocatalysis and biocatalysis is surprisingly underrepresented. By combining the best of each world, chemoenzymatic cascades have great potential to perform chemical transformations in high space-time-yields along with excellent selectivity.

Herein, we present sophisticated multi-way chemo-enzymatic cascades studies. The selective, visible light-accelerated photooxygenation of alkanes is firstly achieved using a water-soluble anthraquinone catalyst, the generated carbonyl group is further transformed by various enzymes. Through this chemo-photo-enzymatic cascade enantiopure products are obtained. The feasibility of this concept is demonstrated with 11 different enzymes giving access to 28 products. Additionally, the scope and limitations of this concept are discussed.

8th December 2016, 09.25 – 09.45

#### *Emerging Photoswitches for Functional Systems*

Michael M. Lerch (RUG), Mickel J. Hansen, Wiktor Szymanski; Ben L. Feringa

The use of photoswitches for dynamic control of biological function has received increased attention in recent years. New classes of photoswitches are emerging: e.g. donor–acceptor Stenhouse adducts (DASAs). To employ them to functional systems, an in-depth understanding of their behavior is required. Herein, we present investigations towards the DASA photoswitching mechanism. The insights allow tuning of photoresponsive properties, especially towards photoswitching under physiological conditions. We also present a novel approach that allows for the first time orthogonal control of two independent photoswitches in the same solution. This approach provides exciting opportunities for photopharmacology and functional control in complex systems.

8th December 2016, 09.45 – 10.05

#### *Development of batch and flow visible light photocatalytic methodology for application in chemical biology*

Cecilia Bottecchia (TU/e), Volker Hessel, Timothy Noel

Photoredox catalysis is emerging as a new and powerful tool in synthetic organic chemistry to facilitate photochemical reactions by means of visible light. As part of our interest to develop efficient synthetic tools for chemical biology purposes, we have evaluated the use of visible light photoredox catalysis for efficient and mild cysteine conjugation in peptides and proteins. In this presentation, we will present our progress in this field and demonstrate the potential use of microreactors to accelerate and scale the photochemical process.

## Abstracts parallel speakers 7/8 December

### Auditorium: Lipids as tools

8th December 2016, 09.05 – 09.25

#### *Lipid membrane solubilization and nanodisc formation by the styrene maleic acid (SMA) co-polymer*

Stefan Scheidelaar (UU), Martijn C. Koorengevel, David Swainsbury, Jonas Dörr, Juan Dominguez Pardo, Rienk van Grondelle, Mike Jones, Antoinette Killian

The styrene maleic acid (SMA) co-polymer has gained much attention in the field of lipid bilayer research, because SMA is able to directly solubilize lipid membranes into nanodisc particles (~ 10 nm in size) without the help of detergents. In this way, membrane proteins can be solubilized in their native lipid environment. This opens new options to study protein-lipid interactions and to solubilize, purify, and characterize membrane proteins that are unstable in detergent. Physico-chemical principles that are relevant for efficient solubilization will be addressed as well as applications involving a photosynthetic bacterial reaction center.

8<sup>th</sup> December 2016, 09.25 – 09.45

#### *Lipids: a tool for graphene bionanotechnology*

Lia Macedo Coelho Lima

Chemically defined and electronically benign interfaces are attractive substrates for graphene and other two-dimensional materials. Here, we introduce lipid monolayers as an alternative, structurally ordered, and chemically versatile support for graphene. Crowd surfing of graphene on the lipids resulted in a more ordered monolayer than regions without graphene. The lipids also offered graphene a more uniform and smoother support, reducing graphene hysteresis loop and the average value of the charge neutrality point under applied voltages. Our approach promises to be effective towards measuring experimentally biochemical phenomena within lipid monolayers and bilayers.

8th December 2016, 09.45 – 10.05

#### *Therapeutic liposome nanofactory*

Alicia Soler Canton (TUD),

Phospholipid vesicles, called liposomes, can be used as containers for targeted drug delivery. We envision that the next generation of vectors will be able to sense environment, produce and deliver the therapeutic agents. Here, we co-encapsulated a DNA template and an RNA polymerase inside 200-nm liposomes and triggered internal transcription as a model system for in situ production of therapeutic RNA molecules. The vesicle reactors were immobilized on a glass coverslip and the amount of synthesized RNA (Spinach aptamer) was analyzed in thousands of single liposomes by fluorescence imaging. The interaction of RNA-loaded vesicles with cultured cells was also investigated.



## Abstracts parallel speakers 7/8 December

### Room 82/83: Protein structure I

8th December 2016, 09.05 –09.25

#### *Better protein structure models with homology-based hydrogen bond restraints*

Bart van Beusekom (NKI), Anastassis Perrakis, Robbie P. Joosten

Producing high quality protein structure models from low-resolution crystallographic datasets is difficult. A high-resolution 'reference' model from the Protein Data Bank (PDB) adds extra information to the model refinement process. But why use just one reference when the average protein has 20 homologs in the PDB? We describe an automated method that finds all suitable homologs and uses them to derive position-specific H-bond restraints. If too few homologs are available, backbone and side-chain H-bond restraints are generated using PDB-wide high-resolution data. Applying these restraints in the PDB\_REDO framework gives more plausible low-resolution structure models, for both published and work-in-progress cases.

8th December 2016, 09.25 – 09.45

#### *Disordered proteins in the eyes of a molecular chaperone*

Magdalena Wawrzyniuk (UU), Madelon M. Maurice, Stefan G.D. Rüdiger

The Hsp90 family constitutes the most abundant cytoplasmic molecular chaperone system, which assists late stages of protein folding. Recently, we obtained a structural model of Hsp90 in complex with Tau, an intrinsically disordered protein. This complex reveals how a disordered protein looks like in the eyes of a chaperone. Based on this paradigmatic interaction, we set out to extract general themes of Hsp90 substrate recognition, which aims to provide a general mechanistic view on why and when a molecular chaperone can recognize intrinsically disordered proteins. We developed an algorithm to identify stretches of similar properties in other disordered proteins. Based on this, here we present a bioinformatic tool for screening for potential Hsp90 binding sites among intrinsically disordered proteins. We further tested the predictions experimentally for a subset of substrates. As first target, we focused on the intrinsically disordered scaffold proteins of the destruction complex of the Wnt signaling cascade.

8th December 2016, 09.45 – 10.05

#### *Template-based protein-protein docking exploiting pairwise interfacial residues restraints*

L. Xue (UU), Rodrigues J.P.G.L.M., Dobbs D., Honavar V., Bonvin A.M.J.J.

While many advanced and sophisticated ab initio approaches for modeling protein-protein complexes have been proposed in past decades. Here we present a template-based method that uses conserved interfacial residue pairs as distance restraints (referred to as CA-CA guided docking). We compare it with interface-guided and simple superposition-based modeling approaches. Our results show that, for most cases, CA-CA guided docking outperforms both superposition and AIR-guided docking. The described CA-CA guided docking protocol is based on the HADDOCK platform, which allows users to incorporate additional prior knowledge of the target system to further improve the quality of the resulting models.

## Abstracts parallel speakers 7/8 December

### Room 80/81: Membrane proteins

8th December 2016, 09.05 – 09.25

#### *Mechanism of zinc transport in bacteria*

Artem Stetsenko (RUG), Cornelius Gati, Dirk J Slotboom, Sjors Scheres, Albert Guskov

Zinc is an essential divalent cation, utilized by numerous intracellular enzymes as a part of their catalytic sites but also used as a stabilizing component by many other proteins. Furthermore, zinc can also fulfill the messenger function and is also crucial for the virulence of several pathogens. Intriguingly, the intracellular concentrations of zinc are very low (picomolar range) as it can be toxic, thus the strict regulation of zinc influx/efflux is required. Here we present the structural characterization of a bacterial zinc transporter in different states. This information is essential to draw the possible mechanism of Zn transport in bacteria

8th December 2016, 09.25 – 09.45

#### *Membrane transporters for Vitamin B12: small proteins handling enormous molecules*

Stephan Rempel (RUG), Joana Santos, Dirk Slotboom

Vitamin B12 is an essential compound for the large majority of bacteria, but it can be synthesised only by a few bacterial species. Therefore, membrane transporters must be ubiquitously present. Surprisingly, very little is known about the uptake of this huge molecule (1.35 kDa) by bacteria. Using a combination of microbiological screens, protein purification and biophysical characterisation we present the first overview of vitamin B12 transporters in bacteria. The membrane transporters are surprisingly small compared to the substrate, raising numerous questions about the transport mechanism.

8th December 2016, 09.45 – 10.05

#### *Towards the adaptation of rhodopsin proton-pumps using retinal analogs and directed evolution*

Srividya Ganapathy (LEI), Que Chen, Jeroen van der Steen, Huub J.M. de Groot, Klaas J. Hellingwerf, Willem J. de Grip

Proteorhodopsins are seven-trans-membrane-helix proteins, which function as light driven proton pumps in many unicellular organisms. They use all-trans retinal as a ligand and naturally absorb maximally between 520-540 nm. We were able to red-shift the absorbance maximum of two proteorhodopsins up to 80 nm using analogs of retinal. One analog induces spectral shifts up to 60 nm, while retaining significant proton pumping capacity. To optimally combine this with mutagenesis, we have constructed a novel directed-evolution set-up, which allows generating a library of proteorhodopsin mutants with simultaneously screening for spectral shifts and proton pumping ability.

## Abstracts parallel speakers 7/8 December

### Room 65: RNA Biology

8th December 2016, 09.05 – 09.25

#### *Quantitative analysis of gene and protein expression in single-cells*

Jan P. Gerlach (RU), Klaas W. Mulder

Single-cell RNA sequencing provides expression profiles for each cell within a certain population. However, it does not provide us with information on the level of proteins or the events triggered by extracellular signaling molecules. We developed the RAID (RNA and Immuno-Detection) technology that uses antibodies conjugated to polyadenylated RNA-barcodes to simultaneously measure global mRNA expression profiles, as well as levels of approximately 100 proteins and their post-translational modifications from single cells.

8th December 2016, 09.25 – 09.45

#### *Cyclophilin inhibitors cyclosporin A and Alisporivir block the replication of a broad range of nidoviruses*

Clara C. Posthuma (LUMC), Adriaan H. de Wilde, Jessika C. Zevenhoven-Dobbe, Corrine Beugeling, Linda Boomaars-van der Zanden, Eric J. Snijder

Outbreaks of the zoonotic SARS- and MERS-coronaviruses have highlighted the potentially lethal consequences of nidovirus infections in humans. Cyclosporin A (CsA), an inhibitor of cyclophilins (CyPs; chaperones of protein folding) blocks nidovirus replication. Replication of the model nidovirus equine arteritis virus (EAV) depends on cellular CypA and CsA treatment affects RNA synthesis directly, presumably by blocking an interaction of CypA with a subunit of the viral replication complex. EAV resistance to CsA treatment is linked to mutations in the viral transmembrane protein nsp5, which may directly link CypA and the viral replication machinery.

8th December 2016, 09.45 – 10.05

#### *Towards an RNase MRP activity assay*

Merel Derksen (RU), Ger J.M. Pruijn

RNase MRP is an essential endoribonuclease, composed of an RNA molecule and 7-10 proteins in a ribonucleoprotein (RNP) complex. Mutations in the RNA component of RNase MRP cause cartilage hair hypoplasia, a disease characterized by short-limbed dwarfism. We aim at gaining insight in the effects of these mutations on RNase activity and RNP composition. Due to the high structural similarity to RNase P, immunoaffinity purification from cell lysates will not result in purified RNase MRP. Therefore, we are developing a technique based upon the streptavidin binding S1m RNA aptamer to obtain catalytically active RNase MRP (and RNase P) complexes.

## Abstracts parallel speakers 7/8 December

### Room 55-57: Analytical Tools II

8th December 2016, 11.05 – 11.25

#### *Enhanced flow control in easily fabricated paper-microfluidic devices*

Nurul Nadiah Hamidon (RUG), Gert Salentijn, Yumiao Hong, Jean-Paul S.H. Mulder, Elisabeth Verpoorte

The hallmark of paper microfluidics is passive fluid transport by capillary action through channels defined by hydrophobic patterning. However, performing reactions controllably in paper is a challenge. Not only are sample and reagents prone to dilution due to large eluent volumes, but they also often exhibit retention on paper, leading to incomplete or even no mixing. To impart greater flow control to these devices, functions like valving and mixing can be patterned into device surfaces to ultimately realize diagnostic applications. This presentation will focus on examples from our labs which could lead ultimately to easy-to-use analytical applications for paper microfluidics.

8th December 2016, 11.25 – 11.45

#### *Immobilized enzyme reactors in analytical chemistry*

B. Wouters (UvA),

Our progress on the design of a microfluidic immobilized-enzyme reactor will be presented. Compared to in-solution digestion, higher enzyme-to-substrate ratios can be achieved by the use of an IMER, leading to higher efficiencies and shorter digestion times in the range of minutes. Depending on the application, specific enzymes (e.g. for proteins or biodegradable polymers) were immobilized on polymer monolithic materials. These monoliths were prepared in-situ in microfluidic channels after which the surface was functionalized post-polymerization. Incorporation of the immobilized-enzyme reactor in a modular microfluidic platform with low dead-volume connections, allowed for in-line implementation of the reactor in an LC×LC workflow.

8th December 2016, 11.45 – 12.05

#### *Surface acoustic wave MS: extremely fast highly sensitive molecular analysis*

Alina Astefanei (UvA), Petra Jansen, Klaas Jan van den Berg, Maarten van Bommel, David Goodlett, Erik Nilsson, Garry Corthals

Surface acoustic wave nebulisation (SAWN) is a new ionisation technique producing similar ions to ESI. The MS spectra are rich in molecular information with minimal molecular fragmentation, less than ESI. We have developed a suite of rapid and sensitive methods that when compared to UPLC-PDA or LC-MS, the total analysis time is at least 25x quicker, and the sample size is easily reduced by a factor of 10, or more. Additionally, sample preparation can be reduced from several hours to several minutes. We will explain the simple instrumental SAWN setup and review numerous ultrafast analyses ranging from human samples to bacteria, dyes, original paint materials, and forensics applications.

## Abstracts parallel speakers 7/8 December

8th December 2016, 12.05 – 12.25

*Integrating MS-based approaches with cryo-EM defines the structural basis of cyanobacterial circadian timekeeping*

Philips Lössl (UU), Joost Snijder, Jan Michael Schuller, Anika Wiegand, Ilka M. Axmann, Jürgen M. Plitzko, Friedrich Förster, Albert J. R. Heck

The cyanobacterial circadian clock is a popular system to study the molecular principles of the daytime-dependent timing of biological processes. Its key feature is the rhythmic auto-phosphorylation and -dephosphorylation of KaiC, which is achieved through transient interactions with KaiA and KaiB. The structural basis of these circadian oscillations, however, is largely unknown. Here, we elucidate the circadian clock architecture based on pseudo-atomic models of the KaiCB and KaiCBA complexes that were obtained by a hybrid approach combining native mass spectrometry (MS), crosslinking-MS, hydrogen/deuterium-exchange-MS and high-resolution cryo-electron microscopy (EM).

## Abstracts parallel speakers 7/8 December

### Boszaal: Analytical applications in life sciences

8th December 2016, 11.05 – 11.25

#### *Protein corona on nanoparticles analyzed by molecular barcodes*

Junhong Yan (TU/e), Luc Brunsveld, Menno W.J Prins

Nanoparticles are widely used in diagnostics due to their large surface area and versatile biofunctionalization. However, nanoparticles are known to attract proteins that form a corona around the nanoparticles when used in a complex matrix, which reduces the biological activity and can cause aggregation among particles. Proteomics studies have analyzed the overall protein composition of coronas on nanoparticles, but not the protein-protein interactions and cooperative effects within coronas. We have developed CoronaTag, a DNA-assisted protein analysis technology wherein proteins are labeled with DNA barcode tags. Protein-protein interactions within the corona are analyzed by ligating proximal barcodes, which reveals protein-protein co-localizations.

8th December 2016, 11.25 – 11.45

#### *In-depth pulsed SILAC/AHA labeling and phosphoproteomics study of the molecular events underlying mGluR-LTD*

Renske Penning (UU), Charlotte AGH van Gelder, Harold D MacGillavry, Casper C Hoogenraad, Albert JR Heck, AF Maarten Altelaar

At neuronal synapses, activation of metabotropic glutamate receptors (mGluR1/5) triggers a form of long-term depression (mGluR-LTD) that relies on new protein synthesis and the internalization of AMPA-type glutamate receptors (AMPA-Rs). Dysregulation of these processes has been implicated in the development of mental disorders such as autism spectrum disorders (ASD).

Rat hippocampal neurons were stimulated with the mGluR1/5 agonist DHPG and harvested at different time points. A highly sensitive phosphoproteomics workflow was applied to study the phosphoproteome. Newly synthesized proteins upon stimulation were enriched and analyzed by applying a pulsed SILAC and AHA-LC-MS strategy. The response was compared with neurons with reduced expression of the ASD-linked Shank proteins.

8th December 2016, 11.45 – 12.05

#### *Cord blood metabolomics: studying in utero HIV-cART exposure in uninfected infants compared to controls*

Johannes C. Schoeman (LEI), Gontse P. Moutloatse, Amy C. Harms, Rob J. Vreeken, Theo W. Kuijpers, Carools J. Reinecke, Ruud Berger, Thomas Hankemeier, and Madeleine J. Bunders

Although, combination antiretroviral therapy (cART) has reduced the risk of mother-to-child transmission of HIV, there are concerns regarding adverse effects in infants following in utero cART exposure. Using comprehensive targeted metabolomics analyses of cord blood plasma, we investigated the impact of in utero cART-HIV exposure on the infant metabolome. The lipid profile was significantly altered in cART-HIV-exposed infants with dysregulated triglyceride, phospholipid and lysophospholipid levels as well as increased oxidized lipids alluding to mitochondrial dysfunction. Finally, the alterations in different lipid metabolites were associated with increased levels of pro-inflammatory cytokines IL-1 $\beta$  and IP-10 respectively, revealing immunological consequences upon exposure.

## Abstracts parallel speakers 7/8 December

8th December 2016, 12.05 – 12.25

### *Antimicrobial activity of volatile organic compounds (VOCs) produced by Streptomyces*

Mariana Avalos (*LEI*), Paolina Garbeva, Jos Raaijmakers, Gilles P. van Wezel

VOCs are small low molecular weight molecules that are readily dispersed through the air. They are widely produced by *Streptomyces* bacteria but poorly studied in terms of their bioactivity. In this study we selected strains for their ability to produce VOCs that inhibit the growth of bacterial cells. The VOC metabolome was analyzed by GC-MS and our results indicate that the antimicrobial activity involves more than one compound, with terpenes being the most abundant compounds. Mode of action studies revealed that VOCs likely target the membrane and that VOCs may lead to alteration of the pH, which increases their bioactivity.

## Abstracts parallel speakers 7/8 December

### Room 63/64: Synthetic Methodology

8th December 2016, 11.05 – 11.25

#### *Fast Cross-Coupling Reactions with Organolithium Reagents*

Dorus Heijnen (RUG),

In the everlasting search for cheaper and more environmentally friendly cross-coupling methods, the use of organolithium reagents provides crucial advantages over traditional organometallics (B/Sn/Zn/Mg) used in these key C-C bond forming reactions. Recent advances with electron rich palladium and nickel complexes have led to increased reactivity and functional group tolerance, and have paved the way for its application. The (diastereoselective) synthesis of the neurotrophically active Mastigophorene A, induced by a point to axial chirality transfer, was achieved by means of a bulky carbene (Pd-PEPPSI) complex. Further application was demonstrated by the successful synthesis of radiolabeled COX-2 inhibitor [11C]-Celecoxib.

8th December 2016, 11.25 – 11.45

#### *Unprecedented phosphinidene transfer reactions from carbene-phosphinidene adducts*

Tetiana Krachko (VU), Mark Bispinchoff, Hansjörg Grützmacher, J. Chris Slootweg

Phosphinidenes are convenient precursors for the synthesis of organophosphorus compounds. Although carbene adducts of phenylphosphinidene (NHC=PPh) have been known for more than a decade, there are no examples that describe the transfer of the phenylphosphinidene fragment from any of the carbene-phosphinidene adducts. Herein, we present the reactivity of MeNHC=PPh toward organic electrophiles that results in phenylphosphinidene transfer reactions. We also show that the reactions can be tuned by the employment of ZnCl<sub>2</sub>. In addition, the reaction pathway of these PhP-transfer reactions is proposed based on DFT calculations as well as the determination of crystal structures of intermediates and products.

8th December 2016, 11.45 – 12.05

#### *Bidentate Ligands-Promoted Palladium-Catalyzed C-H Functionalization*

Kananat Naksomboon (UvA), M. Ángeles Fernández-Ibáñez\*

Metal-catalyzed C-H functionalization is a highly attractive strategy to obtain complex molecules since no preactivation of the starting materials is required. However, the low reactivity of the C-H bond and the low selectivity observed in molecules that contain diverse C-H bonds hampers the broad applicability of this strategy in organic synthesis. An ideal approach to overcome these limitations is by using ligands. Herein, we present the discovery of novel bidentate ligands able to increase the reactivity and selectivity in several C-H functionalization reactions.



## Abstracts parallel speakers 7/8 December

8th December 2016, 12.05 – 12.25

### *Selective functionalization of aromatic heterocycles through hydroamination of alkoxyallenes*

Ivan Bernar (*RU*), Daniel Blanco-Ania, Floris P.J.T. Rutjes

Chemical selectivity, favorable atom economy and asymmetric induction are important targets in developing chemical processes. Recently, we have developed highly effective Pd-catalyzed protocols for the hydroamination of alkoxyallenes with a wide scope of aromatic heterocycles containing nucleophilic nitrogen atoms leading exclusively to branched aromatic derivatives in high yields (up to 95%) and enantiomeric excesses (up to 92%). A new Pd-mediated mechanism will be proposed based on DFT calculations of the process, thereby contributing to a further understanding of transition metal catalysis.

## Abstracts parallel speakers 7/8 December

### Room 58: Enzymology I

8th December 2016, 11.05 – 11.25

#### *Challenges in targeting bi-substrate enzymes: A histone acetyltransferase KAT8 case story*

Hannah Wapenaar (RUG), Frank J. Dekker

Histone acetyltransferases (HATs) are enzymes implicated in diseases such as cancer or inflammatory diseases. Inhibitors of these enzymes could function as therapeutic agents, but a large gap remains between the in-vitro activity of current inhibitors, and their potential use as therapeutic agents. One of the challenges encountered with HAT inhibitors is the lack of potency and selectivity. Calculation of the assay independent inhibitory potency ( $K_i$  values) from  $IC_{50}$  values is crucial for reproducible determination of potency and selectivity. Therefore, we present novel inhibitors of the HAT subtype KAT8 and the kinetic evaluations which enable the calculation of their  $K_i$  values.

8th December 2016, 11.25 – 11.45

#### *Chemoproteomic profiling of the serine hydrolase interaction landscape of the fatal drug BIA 10-2474*

Antonius Janssen (LEI), Annelot C.M. van Esbroeck, Marc P. Baggelaar, Hui Deng, Marco Allarà, Filomena Fezza, Marjolein Soethoudt, Elliot D. Mock, Bogdan I. Florea, Luciano De Petrocellis, Herman S. Overkleeft, Chris I. De Zeeuw, Vincenzo Di Marzo, Mauro Maccarrone, Mario van d

In January 2016, a fatal French drug trial with fatty acid amide hydrolase (FAAH) inhibitor BIA 10-2474 left one volunteer dead and four others hospitalized with symptoms similar to stroke. FAAH degrades long chain fatty acid amides, including the endocannabinoid anandamide. It is thought that BIA 10-2474's off-targets are responsible for the toxicological findings, but its protein interaction landscape is currently unknown. Here, we show, in a comparative chemical proteomics setting with human brain proteomes that BIA 10-2474 targets FAAH, but also unexpectedly inhibits  $\alpha,\beta$ -hydrolase domain-x (ABHD-x), while leaving 25 other identified brain serine hydrolases unaffected.

8th December 2016, 11.45 – 12.05

#### *Design and Synthesis of Bioisosteres of Acylhydrazones as Stable Inhibitors of the Aspartic Protease Endothiapepsin*

Dr. Varsha R. Jumde (RUG), Dr. M. Mondal, Roos C.W. van Lier, M.Yağız Ünver, Prof. Dr. A. K. H. Hirsch

The class of aspartic-proteases plays a causative role in numerous diseases including hypertension, amyloid disease, malaria and AIDS. Endothiapepsin belongs to the family of pepsin-like aspartic-proteases and is a convenient model enzyme. In previous studies, we identified acylhydrazones as inhibitors of endothiapepsin.<sup>1</sup> However, under acidic conditions, acylhydrazones are prone to hydrolyse into aldehydes and toxic hydrazides. Therefore, the design and synthesis of bioisosteres of acylhydrazones is an important step towards the next generation of drugs. We synthesized bioisosteres and determined their biological activity using a fluorescence-based inhibition assay, demonstrating that several bioisosteric replacements are possible without affecting the inhibitory activity.

8th December 2016, 12.05 – 12.25

## Abstracts parallel speakers 7/8 December

*Biophysical interrogation of small-molecule binding to parasitic and human phosphodiesterases (PDEs)*

A.R. Blaazer (VU),

Fragment hit optimization by growing into target-specific binding regions while optimizing ligand selectivity requires a detailed understanding of molecular interactions. A combination of design, synthesis, biochemical and biophysical data, including X-ray crystallography analysis of ligand-protein complexes, can lead to new molecular insights. We apply these approaches to develop inhibitors for parasite phosphodiesterases (PDEs), e.g., from *Trypanosoma brucei*, the causative agent of African sleeping sickness. Our work validates a parasite-specific pocket as a key driver of compound selectivity for TbrPDEB1 over human PDEs. These studies reveal how subtle differences in ligand and protein structure influences compound activity and target binding characteristics.

## Abstracts parallel speakers 7/8 December

### Parkzaal: Supramolecular Chemistry II

8th December 2016, 11.05 – 11.25

#### *Towards synthetic supramolecular intracellular signalling events using self-assembling bipyridine-discotic amphiphiles*

San van Dun (TU/e), Lech-G. Milroy, Christian Ottmann, Luc Brunsveld

The specificity and sensitivity with which proteins function in the cell is facilitated by their compartmentalization in organelles, cell membrane co-localization or via the use of proteins scaffolds. Inspired by the latter, self-assembling supramolecular bipyridine-discotic amphiphiles are under investigation in our group as a dynamic and responsive platform for synthetically engineered interactions between proteins in the cell. This presentation summarizes the results of our efforts thus far, including a discussion of the chemical synthesis and self-assembly properties of the functionalized discotics as well as results from studies on the discotics' cellular uptake mechanisms and localization in cells.

8th December 2016, 11.25 – 11.45

#### *Self-assembled nanoreactors based on the cowpea chlorotic mottle virus capsid*

Lise Schoonen (RU), Roeland J.M. Nolte, Jan C.M. van Hest

The study of catalytic behaviour in small nanocompartments is crucial for understanding biocatalytic processes. To this end, it is useful to encapsulate catalysts in nanocages and study their kinetics. We have utilized the cowpea chlorotic mottle virus (CCMV) capsid to study the catalytic activities of various catalytic moieties, such as enzymes, catalytic peptides, organocatalysts and DNA-based organometallic catalysts. In order to encapsulate these cargoes, we have developed and utilized different types of covalent encapsulation strategies for efficient cargo loading in the virus capsids.

8th December 2016, 11.45 – 12.05

#### *Supramolecular signalling platforms; 14-3-3 proteins as a scaffold*

Anniek den Hamer (TU/e), Lenne Lemmens, Maarten Merkx, Christian Ottmann, Tom de Greef, Luc Brunsveld

Synthetic signalling platforms for the basis for understanding signalling in the cell and provide an entry to complement the cell with novel bottom up functionalities. Here we show how we use 14-3-3 proteins as ideal scaffolds for the bottom-up design of signaling processes. The 14-3-3 protein in interplay with small molecules is used to control and switch signal transduction as illustrated via caspase activation.

## Abstracts parallel speakers 7/8 December

8th December 2016, 12.05 – 12.25

*A protein specific effect of amyloid micronetworks for cartilage tissue engineering*

Maurice van Dalen (UT), Mireille Claessens, Janine N. Post

Several proteins self-assemble into amyloid fibrils with collagen-like strength that form hydrogel-like micronetworks. These micronetworks mimic the extracellular matrix of cartilage. Therefore, we hypothesized that amyloid micronetworks are a potential scaffold material for cartilage tissue engineering.

Self-assembly of the proteins  $\alpha$ -synuclein,  $\beta$ -lactoglobulin, and lysozyme into amyloid micronetworks was confirmed spectroscopically. These micronetworks influenced cartilage cell gene expression and metabolic activity, but the cells remained viable. 3D cultures of cells with networks showed that only lysozyme increased cartilage extracellular matrix formation.

Our results indicate that, depending on the protein used, amyloid micronetworks are a potential scaffold material for cartilage tissue engineering.

## Abstracts parallel speakers 7/8 December

### Auditorium: Biomembranes & Transport

8th December 2016, 11.05 – 11.25

#### *Yeast devoid of the essential membrane lipid phosphatidylcholine*

Xue Bao (UU), Amir Homavar, Martijn Koorengel, Marian Groot Koerkamp, Muriel Mari, Willie Geerts, Ies Nijman, Frank Holstege, Christian Klose, Toon de Kroon

Phosphatidylcholine (PC) is an abundant and essential membrane lipid in the vast majority of eukaryotes. PC synthesis in a yeast *cho2Deltaopi3Delta* mutant that lacks the methyltransferases converting phosphatidylethanolamine into PC, depends on exogenous supply of choline. We isolated *cho2Deltaopi3Delta* suppressor clones that lost the auxotrophy for choline and grow happily in the complete absence of PC (or PC substitute). The phenotypic hallmarks of the first PC-free eukaryote will be presented. Whole genome sequencing revealed that the suppressors acquired 2n-1 aneuploidy with monosomy of one particular chromosome. Research is underway to identify the gene(s) and the mechanism enabling life without PC.

8th December 2016, 11.25 – 11.45

#### *Lipids activate SecA for high affinity binding to the translocon*

Sabrina Koch (RUG), Janny de Wit, Iuliia Vos, Jan Peter Birkner, Pavlo Gordiichuk, Antoine M. van Oijen and Arnold Driessen

Protein translocation across the bacterial cytoplasmic membrane is an essential process catalyzed predominantly by the Sec translocase. This system consists of the membrane-embedded protein-conducting channel SecYEG, the motor ATPase SecA, and the heterotrimeric SecDFyajC membrane protein complex. The exact mechanism by which SecA mediates translocation is poorly understood. Previous studies suggest that anionic lipids are essential for SecA activity and that the N-terminus of SecA is capable of penetrating the lipid bilayer. The role of lipid binding, however, has remained elusive. By employing differently sized nanodiscs reconstituted with single SecYEG complexes and comprising varying amounts of lipids, we establish that SecA gains access to the SecYEG complex via a lipid-bound intermediate state, whilst acidic phospholipids allosterically activate SecA for ATP-dependent protein translocation.

8th December 2016, 11.45 – 12.05

#### *Insights on the transport mechanism of energy-coupling factor transporters using multiscale molecular dynamics simulations*

I. Faustino (RUG), A. Guskov, D.J. Slotboom, S.J. Marrink

Energy-coupling factor (ECF) transporters are responsible for the uptake of micronutrients, such as vitamins, metals or amino acids, in bacteria and archaea. It is suggested that after the substrate binds to one of the subunits of these transporters (S-component) in the extracellular side of the membrane, the ligand-bound protein complex topples over towards the cytosolic side to bind the energy coupling subunits (EcfT, EcfA and EcfA'). In order to examine the physical basis of this mechanism, we have studied the dynamic features of the apo and the holo forms of the folate-specific S-component using multiscale molecular dynamics simulations. The findings obtained in this study shed light on the initial steps of the mechanism of this ATP-binding cassette transporters family.

## Abstracts parallel speakers 7/8 December

8th December 2016, 12.05 – 12.25

*Volume regulation and crowding homeostasis in Escherichia coli probed by super-resolution optical microscopy*

Jonas van den Berg (*RUG*), Arnold Boersma and Bert Poolman

Volume homeostasis, and thus maintaining physicochemical parameters such as crowding, ionic strength and pH, is crucial for optimal functioning of the cell. We determined the volumes of the cytoplasm and the periplasm of *Escherichia coli*, using photo-activated localization microscopy (PALM). In slow growing cells, the cytoplasmic volume is decreased, and the periplasmic volume is increased up to three times, along with an upregulation of periplasmic substrate-binding proteins (SBPs) of many ABC transporters. We show that the cell regulates the volume of the cytoplasm and periplasm and maintains crowding homeostasis, which impacts solute transport as shown for the uptake maltose.

## Abstracts parallel speakers 7/8 December

### Room 82/83: Chemical Biology I

8th December 2016, 11.05 – 11.25

#### *Employing peptide-based nucleosome-mimics to dissect the epigenetic read-out of H3K36me3*

Velten Horn (LEI), Nico van Meeuwenoord, Dima Fillipov, Gijs van der Marel, Hugo van Ingen

Post-translational modifications on histones and their reader proteins play a key role in a large variety of changes in chromatin function.

We recently found that the reader protein PSIP1-PWWP binds very weakly to a native K36me3 peptide but strongly to methylated nucleosomes.

To dissect the role of this nucleosomal context and the histone peptide sequence, we studied the binding of PSIP1-PWWP to various designer H3K36me3-peptides by NMR and MST experiments.

H3K36me3 peptides with additional negative charges show a 20-fold increase in binding affinity.

We therefore conclude a strong interaction of nucleosomal DNA with positive charges on PSIP1-PWWP.

8th December 2016, 11.25 – 11.45

#### *Targeting metabolic resistance to proteasome inhibitor therapy*

Esther Zaal (UU), Pieter Langerhorst, Haley C. Baptist, Celia R. Berkers

Proteasome inhibition has emerged as an important strategy for the treatment of cancer, but treatment is hampered by the occurrence of resistance. We embarked on unravelling the metabolic resistance to the proteasome inhibitor bortezomib. To this end, we profiled bortezomib-sensitive and -resistant cell lines, combining steady-state metabolomics screens with metabolic flux studies using stable isotope labelling approaches. Our studies revealed that the metabolic profiles of bortezomib-sensitive and resistant cells differed significantly. In particular, resistant cells were more dependent on the uptake of specific nutrients from their environment, indicating a potential role for nutrient starvation in the treatment of bortezomib-resistant tumours.

8th December 2016, 11.45 – 12.05

#### *Small-molecule stabilization of the binding between 14-3-3 and CFTR*

Loes Stevers (TU/e),

Cystic Fibrosis is a fatal genetic disease, most frequently caused by the retention of the CFTR mutant protein in the endoplasmic reticulum. The binding of the dimeric 14-3-3 protein to the CFTR regulatory domain has been found to enhance CFTR trafficking to the plasma membrane. We characterized this interaction, showing that multiple phosphorylated binding sites in the CFTR regulatory domain are necessary for significant binding with 14-3-3. Additionally, we discovered that stabilizing this interaction increases the amount of CFTR in the plasma membrane, information that we use to search for new trafficking corrector molecules in Cystic Fibrosis therapeutics.



## Abstracts parallel speakers 7/8 December

8th December 2016, 12.05 – 12.25

*Deciphering the mode of action of clinically relevant drugs developed against Cystic Fibrosis*

Bertrand Kleizen (UU), Florence Peters\*, Marjolein Mijnders\*, Ineke Braakman

Current therapeutic strategy to repair Cystic Fibrosis-causing defects in the chloride channel CFTR (an ABC transporter) is to develop novel and better correctors (to improve folding) and potentiators (to improve function). Using a radiolabeling pulse-chase approach in combination with protease susceptibility and domain-specific antibodies, we track folding and assembly of each of the five CFTR domains with time. We determined mode of action of two clinical drugs, the corrector Lumacaftor (VX-809) and the potentiator Ivacaftor (VX-770) and found that both targeted the first transmembrane-spanning domain (TMD1), the most N-terminal domain of CFTR, during folding and assembly.

## Abstracts parallel speakers 7/8 December

### Room 80/81: Protein regulation and networks

8<sup>th</sup> December 2016, 11.05 – 11.25

#### *Targeting the Middle-East respiratory syndrome coronavirus papain-like protease*

Robert C. M. Knaap, Wei Zhang, Ben A. Bailey-Elkin, Brian L. Mark, Sachdev S. Sidhu, Marjolein Kikkert

Middle-East respiratory syndrome coronavirus replication depends on cleavage of the viral polyproteins by internally encoded proteases, one being a papain-like protease (PLpro). This protease is also a deubiquitinating enzyme (DUB) as it removes ubiquitin and ISG15 from cellular proteins. By selective disruption of the DUB activity of PLpro we demonstrated that this activity is employed to suppress host antiviral pathways. PLpro is an important target for the development of antiviral drugs. We identified proteins that highly selectively bind to PLpro and are competitive inhibitors of catalytic activity by blocking recognition of natural substrates, thereby efficiently preventing MERS-CoV infection in cell-culture.

8th December 2016, 11.25 – 11.45

#### *Revealing an essential role for SUMO in cell cycle progression*

Sabine Cuijpers (LUMC), Karolin Eifler, Edwin Willemstein and Alfred Vertegaal

Reversible protein modification by Small Ubiquitin-like Modifiers (SUMO) is essential for eukaryotic life. Upon knockdown of the SUMO E1 or E2 enzymes in human cells, we have observed mitotic problems, including DNA bridges and micronuclei. Interestingly, we found that the motor protein KIF4A, which is involved in mitotic chromosome positioning and bipolar spindle stabilization is SUMOylated. We have confirmed SUMOylation of KIF4A and generated a SUMO-deficient mutant, which we are currently characterizing. We hypothesize that the inability to SUMOylate KIF4A upon E1 or E2 knockdown is (partially) responsible for the observed mitotic problems.

8th December 2016, 11.45 – 12.05

#### *A conserved two-step binding for the UAF1 regulator to USP12*

Shreya Dharadhar (NKI), Marcello Clerici, Willem J. van Dijk, Alexander Fish, Titia K. Sixma

Ubiquitin signaling is regulated by deubiquitinating enzymes (DUB's). The DUB, USP12 is activated by a WD40 repeat protein called UAF1. We obtained the crystal structure of the USP12-Ub/UAF1 complex which shows two potential sites for UAF1 binding. In solution, we observe two-step binding and 1:2 stoichiometry. We find that high affinity binding is responsible for activation, whereas mutations at the low affinity site only promote intrinsic activity of USP12. Our results highlight the interfaces essential for regulation of USP12 activity and show a conserved second binding of UAF1 which could be important for regulatory functions independent of USP12 activity.

## Abstracts parallel speakers 7/8 December

8th December 2016, 12.05 – 12.25

*Resilience in a family of enzymatic reaction networks*

Albert S.Y. Wong (RU),

Living systems exhibit dynamic behavior that arise spontaneously from intricate networks of interactions between many parts in the systems. Some of the remarkable properties lie in their resilience (i.e. restoration ability) to changes in environmental conditions. Despite advances in theoretical and computation framework, reliable application of reductionist strategies is incomplete without a bottom-up construction of complex molecular systems.

I will present a library-oriented strategy for the construction of enzymatic reaction networks that operate under out-of-equilibrium conditions. Using temperature as perturbation probe, I demonstrate why a specific reaction network can be more resilient than other members of the family of networks.

## Abstracts parallel speakers 7/8 December

### Room 65: DNA structure and integrity

8th December 2016, 11.05 – 11.25

*Insertional mutagenesis: Uncovering a novel cellular mechanism of response to extremely low dose ionizing radiation*

Alex Zelensky (EMC), Roland Kanaar

Insertional mutagenesis occurs when extrachromosomal DNA integrates in the host's genome. We discovered that ionizing radiation doses as low as 0.01 Gy, which are in the range of medical CT scans, significantly increase insertion of exogenous DNA, including episomal virus DNA, in the genome of mammalian cells. This, induced integration, but not the background level of insertion, was absolutely dependent on phosphorylation of H2AX but not its known downstream interactors 53BP1 and MDC1. We are dissecting a novel genetically distinct mechanism of extremely low dose DNA damage stimulated integration of episomal DNA into the genome.

8th December 2016, 11.25 – 11.45

*DNA repair pathway choice: small MAD2L2 decides between giants 53BP1 and BRCA1*

Marco Simonetta (NKI), Inge De Krijger, Judit Serrat, Nathalie Moatti, Vera Boersma, Jacqueline J.L. Jacobs

Depending on the cell cycle phase, cells must choose the appropriate pathway for DNA repair, non-homologous end-joining (NHEJ) in G1 and homologous-recombination (HRR) in S/G2. 53BP1 and BRCA1 promote respectively NHEJ and HRR by opposing each other at sites of DNA double-strand breaks. MAD2L2 was recently characterized as a downstream effector of the 53BP1 pathway. Using a combination of proteomic tools, high-throughput screening technologies and candidate approaches, our lab aims to uncover the molecular mechanisms by which MAD2L2 promotes NHEJ by inhibiting HRR in G1 and, vice versa, BRCA1 neutralizes the inhibitory effect of MAD2L2 to promote HRR in S/G2.

8th December 2016, 11.45 – 12.05

*Simulating the mechanisms and rates of transitions between Watson-Crick and Hoogsteen base pairing*

David Swenson (UvA), Peter G. Bolhuis, David W.H. Swenson

DNA duplexes predominantly contain Watson-Crick (WC) base pairs. However, at any time, a non-negligible fraction of base pairs are in the Hoogsteen (HG) hydrogen bonding motif, where the purine base is rotated approximately 180° relative to the WC motif. The conversion from WC to HG alters the conformation of DNA, and may play a role in several processes, including recognition and replication. The transient nature of these transitions hamper thorough experimental investigation. Molecular dynamics simulations complement experimental work by providing insights at very high spatial and temporal resolution. Path sampling methods focus the molecular dynamics effort on the dynamics during a transition, thus avoiding the long waiting times in stable states. We apply two different path sampling techniques to study the transitions between the WC and HG base pairing motifs. Our results reveal that WC to HG conversion can proceed along several mechanistic routes with varying degrees of exposure of the purine, and we compute rates for these processes.

## Abstracts parallel speakers 7/8 December

8th December 2016, 12.05 – 12.25

*Single-molecule imaging reveals switch between spurious and functional ncRNA transcription*

N. Hermans (LEI), J. Huisman, T. Brouwer, G.P.H. van Heusden, J. Griesenbeck and J. van Noort

Selective pull down of nucleoprotein fragments often requires chemical cross-linking to fix the composition and elevated temperatures for hybridization of sequence specific probes. This limits applications that aim to reveal the native structural properties of chromatin fragments. Here we present a method for the purification of nucleoprotein fragments based on their DNA sequence. A biotinylated DNA oligo with several Locked Nucleic Acid (LNA) nucleotides targets a DNA toe-hold, created by enzymatic digestion, which allows for selective purification of specific DNA fragments at room temperature. We employ this method to obtain single-molecule force extension curves of the 18S rDNA from *Saccharomyces cerevisiae*. We further analyze these fragments with mass spectrometry and electron microscopy. These measurements give insight in the heterogeneity in structure and composition of natively assembled chromatin at the single-molecule level.

## Abstracts parallel speakers 7/8 December

### Room 55-57: Imaging & data handling

8th December 2016, 13.55 – 14.15

*Quantitative Real-time Chemical Imaging of Single Particle Reactivity in Dealuminated Zeolite ZSM-5 Crystals*  
Zoran Ristanovic (UU), Alexey V. Kubarev, Johan Hofkens, Maarten B. J. Roeffaers, Bert M. Weckhuysen

Numerous large-scale catalytic processes involve dealuminated zeolites as acid catalysts. Bulk studies have revealed their improved catalytic performance but the spatial heterogeneities and real-time changes in reactivity of zeolite particles are difficult to study on the single particle level. We present a quantitative, 3-D single molecule fluorescence microscopy approach to follow the real-time reactivity of individual zeolite catalyst particles with 20 nm spatial resolution and single turnover sensitivity. By using mildly and severely steamed zeolite ZSM-5 crystals we show that heterogeneous aluminium distribution and dealumination rates have a large impact on the reactivity and accessibility of Bronsted acid sites.

8th December 2016, 14.15 – 14.35

*Application of self-assembled Pd2L4 metallocages in peptide/protein distribution imaging in tissue and drug delivery*

Jiayang Han (RUG), Hjalmar Permentier, Rainer Bischoff, Geny Groothuis, Péter Horvatovich, Angela Casini

Self-assembly metallocages have become pre-eminent drug delivery systems among supramolecular complexes. The 3D structure of the complex can encapsulate a variety of guest entities, for instance the anticancer drug cisplatin. Thus, we reported a novel Pd2L4 metallocages obtained by self-assembly using Pd metal precursors and exo-functionalized bis(pyridyl) ligands. We coupled various types of Pd2L4 metallocages to different ligands such as short-peptide and proteins following two synthetic approaches. The toxicity of Pd2L4 cages was assessed ex vivo in rat-liver tissues. The coupled ligands allow drug targeting and the fluorescent properties of the metallocages can be applied in fluorescence imaging of peptides/proteins.

#### References

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8th December 2016, 14.35 – 14.55

*Positional Isomer Monitoring by Top-down MS/MS*

Andrea M. Brunner (UU), Albert R.J. Heck, Maarten Altelaar, Richard A. Scheltema

Phosphorylation is a key protein regulatory mechanism influencing activity and ability to interact with other proteins. Topdown proteomics of intact proteins has the potential to determine the phosphorylation state, site and hierarchy; also in hyper-phosphorylated proteins. Here we introduce an approach, utilizing high resolution Orbitrap Fusion/Lumos topdown analyses, allowing for the comprehensive characterization of phosphoproteoforms. These proteoforms cannot readily be distinguished on mass alone as each copy contains the same number of phosphorylations at different positions. We utilize ETD fragmentation and advanced bioinformatics approaches to quantify the contribution of each proteoform and their hierarchy in up to 16x phosphorylated proteins.

## Abstracts parallel speakers 7/8 December

8th December 2016, 14.55 – 15.15

### *Towards Single-Cell Omics With Novel Data Fusion Methods For Flow Cytometry*

Gerjen H. Tinnevelt (*RU*), Bart Hilvering, Selma van Staveren, Leo Koenderman, Lutgarde M.C. Buydens, Jeroen J. Jansen

Multicolor flow cytometry (MFC) is a powerful analytical technology for the simultaneous measurement of multiple markers on single cells. In individuals with an immune response, the number of white blood cells with specific marker expression will change. Analysis of all markers together will lead to better identification of such cells. However, the number of markers per measurement is technologically limited. Currently, more markers can only be measured in multiple 'tubes'. We developed novel data fusion methods that uses blocks of markers that were measured in different tubes. This brings flow cytometry considerably closer to the single-cell omics.

#### Acknowledgements:

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## Abstracts parallel speakers 7/8 December

### Boszaal: Supramolecular Chemistry III

8th December 2016, 13.55 – 14.15

#### *Structural Diversity of a Supramolecular Polymer in Water as Revealed by H/D Exchange*

René Lafleur (TU/e), Xianwen Lou, Anja R.A. Palmans, E.W. Meijer

Numerous self-assembling molecules have been synthesized with the aim to mimic both the structural and dynamic properties found in living systems. It remains a challenge, however, to investigate both the nanoscale organization and the dynamic behavior of the molecules without introducing molecular probes. Here we report on the application of hydrogen/deuterium exchange (HDX) mass spectrometry (MS) to unravel the structural dynamics of a synthetic supramolecular polymer in water. A water-soluble benzene-1,3,5-tricarboxamide (BTA) derivative having six exchangeable H-atoms is self-assembled in H<sub>2</sub>O followed by its dilution in D<sub>2</sub>O. The kinetic H → D exchange profiles as measured at different temperatures unveil structural diversity in these supramolecular polymers in water; a notion that has previously not been observed using other techniques. A mechanism of this diversity in exchange behavior and hence the diversity in supramolecular ordering has been proposed.

8th December 2016, 14.15 – 14.35

#### *Threading polymers through covalently linked double porphyrin cavities*

Kathleen Stout (RU), Mathijs Mabeoone, Eline Meijer, Joëlle Klop, Jeroen van den Berg, Paul White, Theo Peters, Hans Elemans, Alan Rowan, Roeland Nolte

Processive enzymes such as DNA polymerase can accurately transfer information from one substrate to another during replication. To better understand their working mechanisms, a synthetic mimic was developed in which two (metal-)porphyrin cavity-containing molecules are covalently linked. This mimic can thread one or two polyTHF chains equipped with a viologen binding station and a blocking group to ensure that the cavity traverses the complete chain before binding on the viologen occurs. We will present detailed threading studies using polymers of different length and in the presence of bridging axial ligands that modify the 3D structure of the double cavity molecule.

8th December 2016, 14.35 – 14.55

#### *Structure and Long-Term Stability of Alkylphosphonic Acid Monolayers on Stainless Steel*

Medea Kosian (WUR), Maarten M. J. Smulders, Han Zuilhof

Surface modification of stainless steel (SS316L) to improve surface properties or durability is an important avenue of research, as SS316L is widely used in industry and science. We studied, therefore, the formation and stability of a series of organic monolayers on SS316L under industrially relevant conditions. In addition, the concept of multivalent attachment was explored as a means to enhance monolayer stability.



## Abstracts parallel speakers 7/8 December

8th December 2016, 14.55 – 15.15

### *Microstructured soft materials using aqueous multi-phase systems*

Serhii Mytnyk (*TUD*), Alexandre Olive, Kartyk Totlani, Sander Oldenhof, Michiel Kreutzer, Volkert van Stijn, Eduardo Mendes, Jan van Esch

Compartmentalization plays an important role in many biological and industrial processes. So far, the level of complexity of cellular compartmentalization remains out of reach, but few useful approaches have been developed. Many of them employ emulsions, microcapsules, liposomes and polymerosomes to isolate the compartments. Unfortunately, such approaches generally require using organic phases to induce structuring, which may be undesirable. This contribution describes the use of immiscible aqueous polymer solutions to create separate aqueous compartments in hydrogel materials. We explored the use of w/w/w emulsions for microfluidic production of hydrogel capsules with liquid cores and for microstructuring of supramolecular hydrogels.

## Abstracts parallel speakers 7/8 December

### Room 63/64: Chemical Biology II

8th December 2016, 13.55 – 14.15

#### *Rational design of mechanism-based retaining glucosidase inhibitors*

Marta Artola (LEI), Liang Wu, Gideon Davies, Jeroen Codée, Gijs van der Marel, Hans Aerts, Herman Overkleeft

Retaining glycosidases process their substrate glycosides via a mechanism involving a covalent enzyme-substrate intermediate. The natural product, cyclophellitol, capitalises on this mechanism by reacting with retaining beta-glucosidases to form a covalent, irreversible bond. It can do so by conformational mimicry of the emerging half-chair oxycarbenium ion that is formed in the glycosidase active site. Closer perusal of the reaction itinerary by which retaining glycosidases process their substrates allows for the design of a conceptually new class of glycosidase inhibitors: cyclical derivatives featuring cyclic sulphates as electrophilic traps. In this presentation the development of these inhibitors and their application in chemical glycobiology studies will be presented.

8th December 2016, 14.15 – 14.35

#### *Diazotransfer reagents to selectively functionalize a protein of interest with azido groups*

Jonas Lohse (RUG), Alexandra Schindl, Bernhard Kuster, Guillaume Médard, Martin D. Witte

Modification of proteins with a non-natural functional group facilitates fundamental studies, such as target identification. We aimed to develop a method that enables functionalization of a target protein with an azide in a complex mixture. We synthesized targeted-diazotransfer reagents by tethering the reagent to a ligand. The resulting reagents rapidly and selectively label of their respective target. To identify the site of modification, a novel clickable and cleavable linker resin was synthesized, which facilitates enrichment of the azide containing peptides and subsequent the analysis. These experiments revealed that the targeted diazotransfer reagents exclusively modify amino groups proximal to the binding site.

8th December 2016, 14.35 – 14.55

#### *Subcellular proteomic mapping by a spatially-restricted arylamine N-acetyltransferase*

Fleur Kleinpenning (RU), Selma Eising, and Kimberly M. Bonger\*

Mapping protein environments in a specific subcellular location is essential to gain detailed insight on local cell dynamics. We have developed a strategy to identify (unknown) protein interactions that is based on a spatially-restricted arylamine N-acetyltransferase (NAT) that activates hydroxamic acid probes to nitrenium ions, which react fast, covalently, and under neutral conditions with nucleophilic residues of neighboring proteins. The labelled proteins can be isolated and identified with the use of established bioorthogonal chemistries and mass spectrometry. Progress on the technology to profile the subcellular dynamics and identify interacting partners of specific proteins is presented.

## Abstracts parallel speakers 7/8 December

8th December 2016, 14.55 – 15.15

*Using bacteria to make improved, nacre-inspired materials*

Dominik Schmieden (*TUD*), Marie-Eve Aubin-Tam, Anne S. Meyer

Nacre, the inner lining of mollusk shells, is a composite material with outstanding material properties which consists of calcium carbonate platelets connected by an organic matrix. We precipitate calcium carbonate by the urea-hydrolyzing action of *Sporosarcina pasteurii*. Poly-gamma-glutamate (PGA), an anionic polymer produced by many *Bacillus* species, serves to mimic the complex organic layers found in natural nacre. We alternate calcium carbonate precipitation and PGA application to produce our final, layered product. Our biologically-produced nacre is a high-performance composite material produced by biological methods, potentially providing more environmentally-friendly and sustainable materials with applications in e. g. construction or medicine.

## Abstracts parallel speakers 7/8 December

### Room 58: Bio-organic Chemistry

8th December 2016, 13.55 – 14.15

#### *Scaffold-assisted peptide cyclizations: a new approach towards functional protein mimics?*

Gaston Richelle (UvA), Henk Hiemstra, J.H. van Maarseveen, P. Timmerman

In this research, an underexposed strategy for cyclization of peptides namely scaffold-assisted peptide cyclizations is highlighted. By reacting a linear peptide with an external scaffold, looped-like structures can be generated that are able to mimic the discontinuous binding sites of structurally complex proteins.<sup>1</sup> A reaction that has been used in this perspective is the CLIPS reaction developed in our lab, which comprises a reaction between cysteine residues in the peptide with a scaffold containing benzylic bromide moieties.<sup>2</sup> Recent results of my PhD project that is focused on combining the CLIPS reaction with an orthogonal ligation technique in order to create multicyclic peptides (e.g. tricyclic peptides) will be discussed.

1 Heinis, C. Nat. Chem. Biol., 2009, 5, 502–507.

2 Timmerman, P. Chembiochem, 2005, 6, 821–824.

8th December 2016, 14.15 – 14.35

#### *Chemical modifications of aminoglycoside antibiotics to combat bacterial resistance*

Nabil Tahiri (RUG), Andreas A. Bastian, Martin D. Witte, Adriaan J. Minnaard

The continuous emergence of antimicrobial resistance is causing a threat on a global scale. In particular, the use of aminoglycoside antibiotics, broad-spectrum antibacterials of last resort, is limited due to bacterial resistance. One of the major resistances to aminoglycosides is caused by O-phosphotransferase, enzymes which occur predominantly in multi-drug resistant *Escherichia coli*, *Enterococcus* species, *Staphylococcus aureus*, and *Mycobacterium tuberculosis*. To overcome this resistance, we introduce regioselective modifications of aminoglycoside antibiotics via palladium-catalyzed oxidation and other catalytic reactions. Docking studies and biological evaluation of the semi-synthetic aminoglycosides demonstrates the potential of late-stage regioselective modifications as a tool in tackling multidrug-resistant bacteria.

8th December 2016, 14.35 – 14.55

#### *Unprecedented Highly Stereoselective Radiosynthesis of Carbon-11 Labeled Small Peptides for PET Imaging*

A. Pekosak (VUMC),

To advance the application of peptides as PET-tracers we developed a carbon-11 (half-life = 20min) labeling strategy for peptides maintaining their native structure. N-terminal Schiff base-activated tetrapeptides were regio- and stereoselectively alkylated with [11C]benzyl iodide by unexplored radiochemistry methodology utilizing Cinchona alkaloids. This new stereoselective radiosynthetic method afforded pure H-D-[11C]Phe-D-Trp-L-Lys-L-Thr-OH in a 94±2% diastereomeric excess, high radiochemical conversion of 79±6% and an isolated radiochemical yield of 34±6%, via a 5-step radiosynthesis procedure within 46 minutes. This unique approach allows the radiosynthesis of complex 11C labeled peptides for PET imaging studies.

## Abstracts parallel speakers 7/8 December

8th December 2016, 14.55 – 15.15

### *Tetrameric NGR peptide as molecular imaging agent of neovascularization after myocardial infarction*

Ingrid Dijkgraaf (UM), Geert Hendrikx, Tilman M. Hackeng, Mark Post, Dennis Suylen, Felix Mottaghy, Ingrid Dijkgraaf

Angiogenesis plays an important role after myocardial infarction (MI) in partial restoration of blood perfusion. CD13 is selectively expressed on angiogenic endothelium and binds tripeptide motif cNGR. NGR was synthesized, cyclized using native chemical ligation and coupled to a tetrameric scaffold containing a thiaproline (Thz). The sulfhydryl group of Thz was deprotected and reacted with maleimide-DTPA. Resulting DTPA-[SMCC-NGR]<sub>4</sub> was radiolabeled with <sup>111</sup>InCl<sub>3</sub> and angiogenesis after MI was visualized in combination with <sup>99m</sup>Tc-sestamibi in dual-isotope micro-SPECT imaging in a mouse model of MI. Dual-isotope SPECT visualized angiogenesis in the border zone of infarcted myocardium and allowed monitoring of perfusion improvement simultaneously.

## Abstracts parallel speakers 7/8 December

### Parkzaal: Enzymology II

8th December 2016, 13.55 – 14.15

#### *Structural basis of steroid binding and selective oxidation by P450 mono-oxygenase CYP109E1*

Ilona K. Jóźwik (RUG), Flora M. Kiss, Lukasz Gricman, Ammar Abdulmughni, Elisa Brill, Josef Zapp, Juergen Pleiss, Rita Bernhardt and Andy-Mark W.H. Thunnissen

Cytochrome P450 monooxygenases (P450s) are heme-containing monooxygenases catalysing the selective oxidation of unactivated C-H bonds. As biocatalysts they promise a green and cost-effective alternative to complicated chemical synthesis routes for production of drugs or drug precursors. CYP109E1 from *Bacillus megaterium* is a novel steroid-specific P450, which converts testosterone to 16 $\beta$ -hydroxytestosterone. Crystal structures of steroid-free enzyme and of complexes with testosterone and corticosterone were determined at high resolution. Combined structural analysis, site-directed mutagenesis and data acquired from molecular dynamics simulations provide unique insights into the molecular basis of CYP109E1 activity, substrate specificity, and its high regio- and stereoselectivity towards testosterone.

8th December 2016, 14.15 – 14.35

#### *Investigations into the mechanism and substrate specificity of vanillyl alcohol oxidase and eugenol oxidase*

Tom Ewing (WUR), Gudrun Gygli, Willem J.H. van Berkel

Vanillyl alcohol oxidase (VAO) and eugenol oxidase (EUGO) are related flavin-dependent oxidases that catalyse the oxidation of para-substituted phenols. In this project, mutagenesis studies are performed in order to better understand the mode of action of these enzymes and the differences between them. Topics investigated include the molecular determinants and function of the differing oligomerisation states of VAO and EUGO, the molecular mechanism of both their reductive and oxidative half reactions, and the cause of differences in their substrate specificities. Our results further our understanding of these flavin-dependent oxidases paving the way for their use in biocatalytic applications.

8th December 2016, 14.35 – 14.55

#### *Pre-steady state kinetics of redox metalloenzymes*

Batoul Srour (TUD), Marc J.F. Strampaad, W

In order to unravel the catalytic mechanism of redox enzymes under single turnover conditions and on the shortest possible timescale, two new, pre-steady state kinetic instruments have been developed. The first is a rapid-freeze quench instrument (MHQ, microsecond freeze-hyperquenching) that enables trapping of intermediates in a sub-millisecond timescale for characterization by Electron Paramagnetic Resonance, low-temperature UV-Vis and resonance Raman spectroscopy. The second is a continuous-flow UV-Vis/Fluorescence spectrometer with a dead time in the order of microseconds. Results on the electron and hydride transfer pathways in enzymes with multiple redox centres such as FeS clusters, flavin and hemes cofactors will be presented.

## Abstracts parallel speakers 7/8 December

8th December 2016, 14.55 – 15.15

*Rapid freeze-quench multi-frequency EPR; The enzymatic reduction of oxygen by small laccase*

Faezeh Nami (LEI), Mykhailo Azarkh, Peter Gast, Gerard W. Canters, Edgar J.J. Groenen

The study of the mechanism of the enzymatic reduction of oxygen by small laccase (SLAC), a multicopper oxidase, presents a challenge for EPR spectroscopy. Following the changes in the X-band spectra on the time scale of minutes suggested the presence of a biradical intermediate, but EPR studies on the millisecond time scale at multiple microwave frequencies turned out necessary to gain insight into the nature of the intermediate.

We developed an easy and efficient way to combine the rapid-freeze-quench (RFQ) technique with multi-frequency EPR up to 275 GHz. We demonstrate the novel procedures for the model reaction of binding azide to myoglobin. Subsequently we discuss the RFQ-EPR study on the SLAC intermediate, and show that the multi-frequency approach allows the full characterization of a crucial intermediate in the reduction of oxygen by this enzyme.

## Abstracts parallel speakers 7/8 December

### Auditorium: Lipids in cell biology

8th December 2016, 13.55 – 14.15

#### *Clathrin assembly regulated by adaptor proteins in coarse-grained models*

Matteo Giani (UT), Wouter K. den Otter, Wim J. Briels

The assembly of clathrin triskelia into polyhedral cages during endocytosis is regulated by adaptor proteins (APs). We have developed coarse-grained models for clathrin and AP2, employing a Monte-Carlo click interaction, to simulate their collective aggregation behaviour. The phase diagrams indicate that a crucial role is played by the mechanical properties of the disordered linker segment of AP. We also present a statistical-mechanical theory for the assembly behaviour of clathrin, yielding excellent agreement with our simulations and experimental data from the literature. Adaptor proteins are found to regulate the formation of clathrin coats under certain conditions, but can also suppress the formation of cages.

8th December 2016, 14.15 – 14.35

#### *Tethering of the peripheral actin cage to phagosomes*

Maksim V. Baranov (RUMC), Martin ter Beest, Alf Honigsmann, Geert van den Bogaart

Actin plays a critical role during the early stages of internalization of pathogenic microbes by immune cells. In this study, we identified a new mechanism of how F-actin is tethered to the surface of phagosomes in human dendritic cells. We found by multi-color super-resolution STED microscopy that the actin-binding protein SWAP70 aligns with the actin cage on the surface of early phagosomes. siRNA knockdown of SWAP70 disrupted phagocytosis and decreased actin polymerization around phagosomes. These data show that SWAP70 tethers the peripheral actin cytoskeleton to phagosomes.

8th December 2016, 14.35 – 14.55

#### *Halotropism re-visited: biochemical fundamentals behind changes in root growth direction during salt stress*

Ruud Korver (UvA), Christa Testerink

To increase tolerance of crops to salinity, we need to know the cellular and biochemical fundamentals behind plant responses to salt. One of these responses is the alteration of root growth away from higher salt concentrations in the soil, which is called halotropism. Clathrin-mediated endocytosis and phospholipid signalling play important roles in the alteration of the flow of the phytohormone auxin which causes this change in root growth direction. We use a combination of plant physiology, biochemistry and mathematical modelling to unravel the cellular mechanisms underlying halotropism.



## Abstracts parallel speakers 7/8 December

8th December 2016, 14.55 – 15.15

### *Temporal Control of Membrane Fusion through Photolabile PEGylation of Liposome Membranes*

Frederick Campbell (LEI), Li Kong, Sven H.C. Askes, Sylvestre Bonnet, Alexander Kros\*

Membrane fusion results in the transport and mixing of (bio)molecules across otherwise impermeable barriers. In this communication, we demonstrate, for the first time, temporal control of targeted liposome-liposome membrane fusion and contents mixing using light as an external trigger. Our method relies on the steric shielding and rapid, photo-induced de-shielding of complementary fusogenic peptides tethered to opposing liposomal membranes. In an analogous approach, we are also able to demonstrate precise spatiotemporal control of liposome accumulation at cellular membranes in vitro.

## Abstracts parallel speakers 7/8 December

### Room 82/83: Protein structure II

8th December 2016, 13.55 – 14.15

#### *Solving the mystery of C1: Structural insights into the first component of complement*

Deniz Ugurlar (UU), Guanbo Wang, Albert J.R. Heck, Piet Gros

Complement system plays a central role in host defense. Therefore, it is crucial to understand the molecular details of the initial steps of complement activation. The first component C1 is a 790-kDa complex, which consists of 6 recognition proteins C1q and a hetero-tetramer of serine proteases, C1r2C1s2. The proteolytic cascade is triggered when C1 binds to antibodies on target surfaces. In this study, we used hexameric antibodies, which can recruit complement very efficiently. We present EM and MS data on the full 1.65-MDa C1-antibody complex, which provide insight into the structural requirements of C1 activation.

8th December 2016, 14.15 – 14.35

#### *The conformational changes that underlie the function of a sorting receptor*

Nadia Leloup (UU), Bert J.C. Janssen

Sortilin is a multi-ligand sorting receptor expressed abundantly in neurons, hepatocytes and white blood cells. Sortilin internalizes binding partners such as growth factors, signaling receptors and enzymes and directs them from the cell surface to their destined location inside the cells. Its dysfunction can lead to diseases ranging from cardiovascular disorders to neurological diseases. The sortilin molecular sorting mechanism is still unclear. We solved crystal structures of the sortilin ectodomain at varying pH. This revealed, that at endosomal pH, Sortilin undergoes an unusual conformational change which enables it to dimerize. We will discuss the molecular details of this rearrangement and its functional implications.

8th December 2016, 14.35 – 14.55

#### *Steroid binding to Autotaxin links bile salts and lysophosphatidic acid signalling*

Willem-Jan Keune (NKI), Jens Hausmann, Ruth Bolier, Dagmar Tolenaars, Andreas Kremer, Tatjana Heidebrecht, Robbie P Joosten, Manjula Sunkara, Andrew Morris, Elisa Matas-Rico, Wouter H. Moolenaar, Ronald Oude Elferink and Anastassis Perrakis.

Autotaxin (ATX) generates lysophosphatidic acid (LPA) and is involved in multiple (patho)physiological processes. ATX has a tripartite active site, combining a hydrophilic groove, a hydrophobic lipid-binding pocket, and a tunnel. We present crystal structures of ATX bound to steroids, including one simultaneously harbouring a bile salt in the tunnel and LPA in the pocket, revealing that bile salts act as partial non-competitive inhibitors attenuating LPA receptor activation. This interplay provides a molecular basis for associating ATX with disorders linked to increased circulating levels of bile salts and served as a basis for synthesizing a new class of ATX inhibitors.

## Abstracts parallel speakers 7/8 December

8th December 2016, 14.55 – 15.15

*Biochemical and Structural analyses of the Parkinson's disease-related LRRK2 RocCOR domain.*

Franz Y. Ho (*RUG*), Susanne Terheyden, Bert Poolman, Alfred Wittinghofer and Arjan Kortholt

Mutations in LRRK2 are the most frequent cause of late-onset Parkinson's disease (PD). LRRK2 belongs to the Roco family, which is characterized by a conserved Roc-COR G-domain tandem. Our previous studies with prokaryotic Roco proteins revealed that Roco proteins belong to the non-canonical class of dimerizing G protein called GADs. Recently, we were able to successfully express and purify human LRRK2 RocCOR. Here we combine the structural and biochemical studies of this recombinant human LRRK2 RocCOR domain and its prokaryotic homologs to further elucidate the kinetics and mechanism of the LRRK2 G domain cycle and its dysfunction in PD.

## Abstracts parallel speakers 7/8 December

### Room 80/81: Single molecule biophysics

8th December 2016, 13.55 – 14.15

#### *Cardiac troponin conformation switching observed on the single molecule level by antibody-targeted nanomechanics*

Christian Moerland (TU/e), Fabiola A. Gutiérrez-Mejía, Leo J. van IJzendoorn, Menno W.J. Prins

Cardiac Troponin (cTn) is a protein complex of which a calcium-triggered conformational change regulates muscle contraction. Here we demonstrate that antibody-based targeting in a sandwich format can be used to record cTn conformation changes at the single molecule level. Nanomechanical changes could be sensitively studied by capturing the cTn between a particle and a substrate, via three independent nanomechanical observables: Magnetic torque tweezers, and translational and rotational Brownian motion. Changes in the  $\text{Ca}^{2+}$  concentration show consistent results in the three observables. This experimental approach opens a new perspective for quantifying nanomechanical properties and analysing conformational changes of native protein complexes. Fabiola A. Gutiérrez-Mejía †,‡, Christian P. Moerland†,‡, Leo J. van IJzendoorn †,‡, Menno W.J. Prins\*, †,‡,§

†Department of Applied Physics, Eindhoven University of Technology (TU/e), Eindhoven, the Netherlands ‡ Institute for Complex Molecular Systems (ICMS), TU/e, Eindhoven, The Netherlands, § Department of Biomedical Engineering, TU/e, Eindhoven, the Netherlands

8th December 2016, 14.15 – 14.35

#### *Fluorescence of fluorophores in lipid bilayers enhanced by gold nanorods*

Biswajit Pradhan (LEI), Thijs J. Aartsma, Gerard W. Canters, Michel Orrit

Fluorescence correlation spectroscopy (FCS) is used to study plasmonic fluorescence enhancement at micromolar concentrations of an emitter. Previously such studies suffered from sticking of the dyes to the substrate and poor quantum yields. A passivating lipid bilayer prevents sticking and allows specific anchoring of probe molecules. Fluorescence traces of emitters in the near field of a gold nanorod exhibit enhanced signals due to their enhanced radiative rate. This promotes the contrast of the FCS function by two orders of magnitude. We show how a lipid bilayer can be used to anchor a dye-labelled protein and obtain an enhanced FCS trace.

8th December 2016, 14.35 – 14.55

#### *Correlative Light and Electron Microscopy imaging of pathogen-phagocyte interactions using bioorthogonal labeling*

Daphne M. van Elsland (LEI), Erik Bos, Abraham J. Koster, Sander I. van Kasteren

We combine bioorthogonal chemistry with correlative light-electron microscopy (CLEM) to follow bacterial degradation in the phagolysosomal system of phagocytic immune cells. We have employed bioorthogonal non-canonical amino acid tagging to incorporate bioorthogonal groups in bacteria and developed a method to label and detect these bioorthogonal groups with CLEM-imaging. This allows us to obtain high resolution information on the subcellular location of degraded bacteria.

## Abstracts parallel speakers 7/8 December

8th December 2016, 14.55 – 15.15

*Single-molecule imaging reveals switch between spurious and functional ncRNA transcription*

Tineke Lenstra (*NKI*), Antoine Coulon, Carson C. Chow, Daniel R. Larson

Genomic data indicates that eukaryotic genomes are ubiquitously transcribed, but the function of non-coding RNAs is largely unknown. In this study, we use simultaneous single-molecule visualization of coding and non-coding transcription at the GAL locus in living yeast to elucidate the role of ncRNA in metabolic decision making. We find that ncRNA transcription prevents transcriptional leakage at the locus under repressed conditions, but also appears during activation with no detectable effect on transcription, highlighting the nuanced roles that ncRNA can play in gene regulation.

## Abstracts parallel speakers 7/8 December

### Room 65: Epigenetics

8th December 2016, 13.55 – 14.15

#### *A maintenance mechanism for histone variant H2A.Z in dynamic promoter nucleosomes*

Tessy Korthout (NKI), Marit Terweij, Deepani Poramba Liyanage, Tibor van Welsem, Iris J.E. Stulemeijer, Hanneke Vlaming, Kitty F. Verzijlbergen, and Fred van Leeuwen

Histone H2A.Z, the major variant of histone H2A, is a conserved player in gene regulation and enriched at regulatory regions characterized by dynamic chromatin states. Together with its biochemical properties, this suggests that H2A.Z is a highly unstable chromatin feature. Here we determined in yeast the genome-wide dynamics of H2A.Z using Recombination-Induced Tag Exchange (RITE) to distinguish old histone proteins from newly synthesized ones. Although new H2A.Z incorporation can in principle occur throughout the cell cycle, it did not occur in G1-arrested cells. In non-replicating cells old H2A.Z was remarkably stable in promoter nucleosomes, which undergo turnover of histone H3 and are expected to evict and replace H2A.Z in the process. SWR1, the ATP-dependent chromatin-remodeling complex known for exchanging nucleosomal H2A for new H2A.Z was found to be responsible for a recycling mechanism maintaining existing H2A.Z. Our findings suggest that information encoded in promoter chromatin is differentially retained during nucleosome disassembly and re-assembly, with H2A.Z being retained and histone modifications on H3 being erased.

8th December 2016, 14.15 – 14.35

#### *Reading the readers of the *P. falciparum* epigenome*

Wieteke Hoeijmakers (RU), Hendrik G. Stunnenberg, Richard Bartfai

In our lab we dissect Plasmodium epigenetic mechanisms, with the ultimate aim to develop epigenetic anti-malarials against this deadly pathogen. To disclose the molecular mechanisms by which epigenetic marks translate into function we set out to identify reader-protein-complexes. Using histone-peptide-pulldown coupled to quantitative-proteomics, we identified a parasite-specific PHD-domain-protein recruiting an atypical SAGA-complex to di-/tri-methylated H3K4-peptides. Furthermore, we discovered multiple bromo-domain-protein-complex being recruited to highly acetylated tails of (amongst others) parasite-unique histone variants H2A.Z and H2B.Z. Importantly, the Plasmodium-specific proteins residing in these complexes could open up a treasure-trove of targets for selective modulation of Plasmodium epigenetic-enzyme-complex recruitment and activity.

8th December 2016, 14.35 – 14.55

#### *Dynamics of Polycomb localisation and abundance in pluripotency*

Guido van Mierlo (RU), Nehmé Saksouk, René A.M. Dirks, Jerome Dejardin, Hendrik Marks

Naïve and metastable embryonic stem cells (ESCs), respectively 2i and serum, possess a distinct epigenome, exemplified by the near absence of DNA methylation in naïve ESCs. We applied total chromatin profiling using mass spectrometry and identified remarkable differences in abundance of major epigenetic complexes, such as Polycomb Repressive Complex 2 (PRC2), on the chromatin. Immunofluorescence, as well as locus purification, revealed that PRC2 partially relocates to pericentric heterochromatin. By affinity purification we also show that the architecture of PRC2 is strongly remodeled. We are currently investigating the role of different subunits in the recruitment of PRC2 to pericentric heterochromatin.

## Abstracts parallel speakers 7/8 December

8th December 2016, 14.55 – 15.15

### *Dynamic and versatile DNA binding of archaeal histones*

Bram Henneman (LEI),

To organize their genomes, archaea express histone proteins that are homologous to their eukaryotic counterparts H3 and H4. Eukaryotic histones are believed to originate from archaeal histones. Unlike eukaryotic histones, which predominantly wrap DNA around an octameric histone core, archaeal histones bind to DNA as dimer, tetramer or larger multimer. Here, we examined the histones from *Methanothermobacter* *thermautotrophicus*. Our biochemical data indicate that tetrameric nucleosome-like structures are formed on high-affinity sites and that higher concentrations drive cooperative aspecific DNA compaction. We propose that aspecific binding is important for genome organization, whereas specific binding serves a function in regulation of transcription.

## General information Poster Presentations

All posters will be on display in either the Diezhal or the Genderhal, which are located next to the congress floor. Please consult the NWO CHAINS App, or the abstractbook on our website ([www.nwochains.nl](http://www.nwochains.nl)) to access the complete poster list and find information about the designated place where to put/find specific posters.

Your personal poster number can be found in the 'poster list' as well as in your confirmation email. The following poster presentation moments are scheduled (for details see poster list):

Posters with odd numbers for ST, SM, CSM, MM, C, CCHK, and PT:

- Tue 6 Dec. 12.25 - 14.00 hrs
- Tue 6 Dec. 15.10-16.00 hrs

Posters with even numbers for ST, SM, CSM, MM, C, CCHK, and PT:

- Tue 6 Dec. 20.00-22.00 hrs

Poster award ceremony for the above mentioned posters:

- Wed 7 Dec. 17.25 hrs

Posters with odd numbers for PR, NA, LB, BMC, DS, SR, MC and AC:

- Wed 7 Dec. 20.15-22.00 hrs

Posters with even numbers for PR, NA, LB, BMC, DS, SR, MC and AC:

- Thu 8 Dec. 10.15 - 11.05 hrs
- Thu 8 Dec. 12.25 - 13.55 hrs

Poster award ceremony for the above mentioned posters:

- Thu 8 Dec. 17.05 hrs

All posters will be exposed as long as possible, so we ask poster presenters to put up their poster immediately upon arrival and remove their poster when leaving the conference. Push pins for attaching your poster to the posterboards will be provided. Additional assistance for poster presenters is available at the information desk in the Kempenhal.

Please note that posters that are not removed by the end of the conference (Thursday 8 December, 17.30) will be removed by NWO. Posters that are removed by NWO cannot be retrieved.

A poster jury will award several prizes to the most outstanding poster presenters. This year will also be the first year to feature a poster prize awarded by the audience. For this award, participants can vote for their favourite poster via the NWO CHAINS app. The poster awards will be announced at the end of the programme of Wednesday 7 December, for posters presented on 6/7 December, and at the end of the programme of Thursday 8 December, for the posters presented on 7/8 December.

Prizes will be awarded according to the 'no show, no prize' principle, therefore make sure that you are present at the award ceremony.



<b>Poster sessions CHAINS 2016 (By poster number)</b> <b>Posters with odd numbers for ST, SM, CSM, MM, C, CCHK, and PT: Tuesday 6 December 12.25 - 14.00 hrs and 15.10-16.00 hrs</b> <b>Posters with even numbers for ST, SM, CSM, MM, C, CCHK, and PT: Tuesday 6 December 20.00-22.00 hrs</b>  <b>Posters with odd numbers for PR, NA, LB, BMC, DS, SR, MC and AC: Wednesday 7 December 20.15-22.00 hrs</b> <b>Posters with even numbers for PR, NA, LB, BMC, DS, SR, MC and AC: Thursday 8 December 10.15 - 11.05 hrs and 12.25-13.55 hrs</b>					
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Analytical chemistry					Wed 7 Dec/Thu 8 Dec
Poster number	First name	Prefix	Family name	Affiliation	Poster title
AC01	Noor		Abdulahussain	UvA	Identification protein kinases from tissue-derived glioblastoma cell lysate by LC-MS/MS
AC02	Oier		Aizpurua Olaizola	VU	Affinity capillary electrophoresis for the assessment of binding affinity of cholera toxin inhibitors
AC03	Erika		Amstalden	VU	Alternative detection and confirmation of non-covalent protein complexes by MALDI-MS
AC04	Alina		Astefanei	UvA	SAWN-MS assays for art, forensics and sustainability
AC05	Andrei		Barcaru	UvA	CHROMAMETRIX: creating new ways of interpreting GCxGC(-MS) data
AC06	Karlijn		Bezemer	UvA	Profiling of TATP using IRMS and GC-IRMS
AC07	Fleur	van	Beek	UvA	Making Analytically Incompatible Approaches Compatible
AC08	Roy		Boonen	TU/e	Polymer-based nanoparticle coatings for molecular biosensing in blood plasma
AC09	Samuel		Confederat	WUR	Evaluation of Translocation Properties of a Gut-on-a-Chip Intestinal Barrier Model
AC10	Charlotte		Croes	UvA	Characterization of natural dyes by comprehensive 2D liquid chromatography
AC11	Irena		Dapic	UvA	Methods for monitoring proteome complexity in human tissues
AC12	André	van den	Doel	RU	Understanding 20th century oil paint chemistry
AC13	Sergio		Fernandez	RUG	Quantitative Tunable Hydrodynamic Chromatography of Polymer Microparticles in Short, Non-uniform Microchannels
AC14	R		Folcarelli	RU	A NOVEL MULTIVARIATE METHOD FOR SELECTION OF IMMUNOLOGICAL CELLS WITH MULTICOLOUR FLOW CYTOMETRY
AC15	Alan Rodrigo		García Cicourel	UvA	Mineral oil analysis in consumer products: Relevance, principles and novel LC, SPE and GC-VUV methods.
AC16	Maciej	M.	Grajewski	RUG	INTEGRATED CELL CULTURE PLATFORM FOR REAL-TIME MONITORING OF ADHERENT CELL CULTURES
AC17	Iris		Groeneveld	COAST	The detection of bacteria in waterborne paints by fluorescence spectroscopy
AC18	Pim	de	Haan	RUG	Fabrication of stretchable, porous membranes for organ-on-a-chip applications
AC19	Rob		Haselberg	VU	Fully compatible and ultra-sensitive micellar electrokinetic chromatography-tandem mass spectrometry using sheathless porous tip interfacing
AC20	Margaryta		Ianovska	RUG	Implementation of Chaotic Microfluidic Mixers in Two-Dimensional Liquid Chromatography
AC21	Rashieda		Jahangier	VU	The search for fusicoccin-like compounds in plant extracts with help of HPLC in combination with MS and nanofractionation
AC23	Abidemi		Junaid	LEI	A human microvascular organ-on-a chip platform to assess circulating factors associated with microvascular destabilization
AC24	Ruben		Kers	UvA	Optimization and development of a second-dimension separation method for the analysis of polymer nanoparticles by comprehensive two-dimensional liquid chromatography
AC25	Koeman		Koeman	RU	MORE RELIABLE MODELS BY CORRECTING FOR INDIVIDUAL VARIATION
AC26	Pieter		Kooijman	UM	Combined plasma and electrospray ionization source for laser ablation electrospray ionization mass spectrometry imaging (LAESI-MSI)
AC27	Valeriia		Kuzyk	VU	CE-MS glycosylation profiling of carcinoembryonic antigen
AC28	Giulia		Lambiase	VU	Intact glycoform characterization of rHu EPO in HSA-containing formulations by HILIC-MS
AC29	Simon		Leygeber	LEI	Improved pre-concentration and separation by depletion zone isotachophoresis
AC30	Olga		Lushchikova	RU	Development of an alarm system for water quality control based on flow cytometry data of algal populations
AC31	Morwarid		Mayar	VU	Development and optimization of an at-line nanofractionation platform with parallel mass spectrometry for identification of plasmin inhibitors and activators in snake venom
AC32	Paul		Miggiels	LEI	Vision-controlled droplet evaporation as performant preconcentration technique for LC-MS metabolomics of volume-limited samples
AC33	Marta		Mourao	UvA	Study of large molecules using on-line Liquid Chromatography × Gas Chromatography-Mass spectrometry
AC34	Amar		Oedit	LEI	Electroextraction coupled on-line to capillary electrophoresis – mass spectrometry: an innovative tool for metabolomic profiling of biomass-limited samples
AC35	Rianne	van	Outersterp	RU	Identification of metabolite biomarkers from body fluids using infrared ion spectroscopy
AC36	Angie	ten	Pierick	VU	Towards robust analysis of human growth hormone by capillary electrophoresis-mass spectrometry – essential considerations
AC37	Bob		Pirok	UvA	OPTIMIZATION OF REACTOR ASSISTED NANOPARTICLE ANALYSIS
AC38	Susanna		Pot	VU	Analysis of antibody charge variants by isoelectric chromatofocusing coupled to native mass spectrometry
AC39	Eva	de	Rijke	UvA	Development of an isotopic traceability tool for the geographical origin of roses
AC40	Liana Sorina		Roca	UvA	STAMP-Separation Technology for A Million Peaks
AC41	Rosilene		Rossetto Burgos	LEI	Towards a better understanding of the molecular mechanism underlying ultra-weak photon emission from biological systems using a metabolomics approach
AC42	Max		Scheepers	TU/e	The (in)stability of nanoparticles in blood plasma: How to quantify at the single-particle level?
AC43	Rickdeb		Sen	WUR	Measuring the Rate of Organic Reactions on Surfaces
AC44	Kathryn		Stevenson	UvA	MOP: Modulation Optimization Program for In-Column-Focusing (ICF)
AC45	Teemu		Suutari	VU	Living Cell Sensing Using Multi-Parametric Surface Plasmon Resonance in Drug Development and Drug Research
AC46	Mimi	den	Uijl	UvA	Analysis of organophosphorus flame retardants in sewage water treatment plant influent and effluent samples
AC47	Gerjen		Tinnevelt	RU	TOWARDS SINGLE-CELL OMICS WITH NOVEL DATA FUSION METHODS FOR FLOW CYTOMETRY DATA
AC48	I.K.		Ventouri	UvA	Understanding aqueous SEC-MS elution and ionization behavior of biomacromolecules
AC49	Thomas		Vijverberg	RU	
AC50	Matthias		Vink	VU	Quantitative analysis of cyclodextrins in human gastric and intestinal fluids by LC-MS/MS
AC51	Markus		Weingarth	UU	Sensitivity-enhanced NMR to study the dynamic of proteins in their native cell membrane
AC52	Cornelius		Willacey	LEI	LC-MS approach to quantify dopamine and its metabolites within cell culture media utilising a novel stabilisation method
AC53	Mengyun		Xu	RUG	A miniaturised protein microarray platform with quantification by internal calibration: Spot-to-spot correction
AC54	Bert		Wouters	UvA	DESIGN OF AN IMMOBILIZED-ENZYME MICROFLUIDIC REACTOR FOR RAPID ONLINE DIGESTION OF VARIOUS NATURAL MACROMOLECULES
AC55	Shengqi		Xiang	UU	High sensitivity (1H)) solid-state NMR approaches applied to complex biomolecules
AC56	Wei		Zhang	LEI	Sheathless capillary electrophoresis-mass spectrometry for metabolic profiling of volume-limited samples
AC57	Xiaoyan		Zhang	LEI	Very Fast DNA Translocation Speed in Graphene Nanodevices
AC58	Adja		Zoumaro-Djajoon	LEI	Oxylipins analysis in interstitial fluid of pancreatic cancer cell model

Poster number	First name	Prefix	Family name	Affiliation	Poster title
<b>BMC01</b>	Can		Araman	LEI	Generation of citrullinated, bioorthogonal antigens to study their impact in rheumatoid arthritis
<b>BMC02</b>	Dowine	de	Bruijn	RUG	Bioorthogonal Metal Catalysis
<b>BMC03</b>	Maarten		Bakker	TU/e	Controlled Drug Delivery from a Supramolecular Injectable Ureidopyrimidinone Hydrogel
<b>BMC04</b>	Jorick		Bruins	WUR	C-terminal labelling of proteins using enzymatic oxidation of tyrosine
<b>BMC05</b>	Hanna		Busch	TUD	The re-evaluation and isolation of a novel Michael hydratase from Rhodococcus rhodochrous ATCC 17895
<b>BMC06</b>	Stefano		Canziani	WUR	Novel lutein extraction from microalgae
<b>BMC07</b>	Shoupeng		Cao	TU/e	Tumor environment responsive block-co-polymer for system bio-reactor and nano-medicine
<b>BMC08</b>	Shreyans		Chordia	RUG	Artificial Metalloenzymes: towards in vivo catalysis
<b>BMC09</b>	Jurriën		Collet	VU	Rapid Synthesis of Synthetically and Biologically Valuable $\alpha$ -Ketospecies Via an Ugi/Oxidative Hydrolysis Sequence.
<b>BMC10</b>	Maurice	van	Dalen	UT	A protein specific effect of amyloid micronetworks for cartilage tissue engineering
<b>BMC11</b>	Liliana		Cozzoli	RUG	Controlling the self-assembly of DNA G-quadruplex micelles
<b>BMC12</b>	Linda		Dijkshoorn	RUG	The creation of a synthetic methylotrophic Bacillus subtilis for the sustainale production of high value chemicals
<b>BMC13</b>	Paul		Dockerty	RUG	Enol-cyclocarbamate, penicillin binding proteins inhibitors and serine hydrolases probes
<b>BMC14</b>	Nienke	van	Dongen	WUR	Spectral analysis of EGFP and mEGFP encapsulated in C3Ms
<b>BMC15</b>	Sam	van	Dun	TU/e	Cellular uptake of Bipyridine-Discotic Amphiphiles
<b>BMC16</b>	Selma		Eising	RU	A new bioorthogonal Carboni-Lindsey reaction with vinylboronic acids
<b>BMC17</b>	Wouter		Engelen	TU/e	Antibody-controlled actuation of DNA-based molecular circuits
<b>BMC18</b>	Robert		Englmeier	UU	Structural investigation of the mammalian mitochondrial translation system using Cryoelectron Tomography
<b>BMC19</b>	Bauke		Gaastra	RUG	Building a Synthetic Cell: Sensing the energy status of lipid vesicle systems
<b>BMC20</b>	Berend		Gagestein	LEI	Probing lipid signaling molecules
<b>BMC21</b>	Mark	de	Geus	LEI	In-vivo bioorthogonal activation of silenced MHC-1 peptide antigens
<b>BMC22</b>	Cora		Gutierrez de Souza	RUG	Artificial metalloenzymes by in vivo incorporation of metal-binding amino acid
<b>BMC23</b>	Simone		Hendrikse	TU/e	Biofunctionalized supramolecular hydrogels for organoid expansion
<b>BMC24</b>	Alberto		Juan Ruiz Del Valle	UT	NMR- STD highlights the binding site of a photo-switch based protein for simultaneous light-triggered ligand release
<b>BMC25</b>	Robin		Klem	UT	Encapsulin as a Platform for Enzyme Delivery
<b>BMC26</b>	Gulistan		Kocer	UT	Biomaterial Supported Lipid Bilayers (BSLBs) as Stem Cell Microenvironments
<b>BMC27</b>	Petra		Krumpochova	UvA	Rapid quenching method for quantitative analysis of intracellular metabolites in Lactococcus lactis.
<b>BMC28</b>	Zeynep		Kurkcuoglu Soner	UU	Pre- and post-sampling conformational changes for protein-protein docking using elastic network modelling
<b>BMC29</b>	Lianne		Lelieveldt	RU	Targeting and Elimination of Autoreactive B cells in Rheumatoid Arthritis
<b>BMC30</b>	Lenne		Lemmens	TU/e	14-3-3 heterodimers as scaffolds for synthetic signaling networks
<b>BMC31</b>	Jonas		Lohse	RUG	
<b>BMC32</b>	Dennis		Lowik	RU	Cell-penetrating peptides with intrinsic cancer cell selectivity
<b>BMC33</b>	Jolien		Luimstra	LUMC	Improved peptide vaccines through chemical modification of HLA-A2-restricted T cell epitopes
<b>BMC34</b>	Ruben		Maaskant	RUG	Bio-orthogonal metalloporphyrin catalyzed modification of lantibiotics
<b>BMC35</b>	Eva		Magdalena Estirado	TU/e	Self-assembled multivalent platforms for protein assembly and cellular targeting
<b>BMC36</b>	Lenny		Meijer	TU/e	Controlling enzymatic actuators using in-vitro DNA-based switchable memories
<b>BMC37</b>	Adrien		Melquiond	UU	Integrative Modeling of the Endoplasmic Reticulum translocon complex
<b>BMC38</b>	Luuk		Mestrom	TUD	Aqueous Asymmetric Oxidation of Unprotected $\beta$ -Amino Alcohols using Alcohol Dehydrogenases
<b>BMC39</b>	Qing		Miao	LEI	Toward the ultimate lanthanoid NMR probe for the study of proteins
<b>BMC40</b>	Irina	S	Moreira	UU	Supervised classification applied to hot-spot detection
<b>BMC41</b>	Linda		Otten	TUD	First steps toward polymerisation in water using lipases
<b>BMC42</b>	Lisanne	van	Oppen	RUMC	Elastin-like Polypeptide Nanoparticles as Tool for Targeted Drug Delivery
<b>BMC43</b>	Linda		Pieper	LEI	BIO-ORTHOGONAL ANTIGENS TO INVESTIGATE ANTIGEN CROSS-PRESENTATION
<b>BMC44</b>	Johan		Pijnenborg	RU	Rational design of sialic acid mimetics to target specific human Siglecs
<b>BMC45</b>	Jan		Pille	RU	Self-assembling nanobodies for nanomedicine
<b>BMC46</b>	Imke		Pijpers	TU/e	Formation of Well-Defined, Functional Nanotubes via Osmotically Induced Shape Transformation of Biodegradable Polymersomes
<b>BMC47</b>	Dimitrios		Poulcharidis	LEI	A Flow Cytometry Assay to Quantify Intercellular Exchange of Membrane Components
<b>BMC48</b>	Aleksandr		Pogodaev	RU	Light control of the enzymatic chemical reaction network.
<b>BMC49</b>	Rindia		Putri	UT	Bacterial encapsulin nanocages as platform for light-responsive protein-based systems
<b>BMC50</b>	Katharina		Rosenbusch	RUG	Characterizing amoebic proteins to study LRRK2 mediated Parkinson's disease
<b>BMC51</b>	Mark	de	Ruiter	UT	From a virus to an enzyme based drug
<b>BMC52</b>	Jurgen		Schill	TU/e	Red-shifted oligomers for sensing and bioimaging
<b>BMC53</b>	Loes		Stevens	TU/e	Stabilization of the interaction between 14-3-3 and CFTR
<b>BMC54</b>	Mikael		Trellet	UU	Integrative Modelling goes HPC/HTC
<b>BMC55</b>	Lara		Villarino Palmaz	RUG	Supramolecular assembly of artificial metalloenzymes
<b>BMC56</b>	Pim	de	Vink	TU/e	Multi-Component Assembly of an 14-3-3/Cucurbit[8]uril Supramolecular Protein Complex
<b>BMC57</b>	Reinder	de	Vries	RUG	Synthesis of N4Py Derivatives Containing Targeting Groups for Tumor Cells
<b>BMC58</b>	Dennis		Wander	LEI	Anthracyclines: anti-cancer treatment without inducing DNA damage?
<b>BMC59</b>	Rong		Wang	UM	To develop instructive scaffolds through additive manufacturing
<b>BMC60</b>	Maike		Wiemann	UT	Switchable Bioactive Ligands for Supramolecular Surfaces
<b>BMC61</b>	Sjors		Wijnands	TU/e	Controlling enzyme activity by modular protein recruitment on supramolecular polymers
<b>BMC62</b>	Li		Xue	UU	Template-based protein-protein docking exploiting pairwise interfacial residue restraints
<b>BMC63</b>	Ying		Zhang	RU	Biological application of polyisocyanopeptide hydrogel
<b>BMC64</b>	Yang		Zheng	VU	Phosphodiesterase Inhibitors as a Potential Treatment for Neglected Parasitic Diseases

Catalysis						Tue 6 Dec/Wed 7 Dec
Poster number	First name	Prefix	Family name	Affiliation	Poster title	
C01	Rohit		Chaudhary	TU/e	CO2-neutral Methanol Synthesis from CO2 and H2 by Smart-Scaled, Reaction Integrated Plasma Process	
C02	Robin		Broos	TU/e	The effect of surface termination on key reactions for Fischer-Tropsch reaction over iron-carbides	
C03	Juan Fernando		Collados	RUG	Asymmetric synthesis of alpha-silylated C-tertiary amines by Cu-catalyzed addition of Grignard reagents to silylimines	
C04	Peter		Deuss	RUG	Lignin derived acetals obtained via acid mediated depolymerization	
C05	Piotr		Gajewski	UvA	Peptide C-terminal activation via Ru-catalyzed enol elongation	
C06	Yuan		Gao	UvA	A europium-based metal organic framework as humidity sensor	
C07	Homer		Genuino	UU	ZrO2 is preferred over TiO2 as support for the Ru-catalyzed hydrogenation of levulinic acid to $\gamma$ -valerolactone	
C08	Andreea		Gheorghe	UvA	Designing chiral metal organic framework for enantioselective catalysis	
C09	Joeri		Hessels	UvA	Porpyrinic MOFs for renewable fuel production	
C10	Aijie		Liu	UT	Viral cage-gold hybrid NPs in flow reactor and their catalytic activity	
C11	Nazila		Masoud	UU	The stability of Au and Au-Ag catalysts for the model hydrogenation and oxidation reactions	
C12	David	Dr.	Martin	UvA	X-ray spectroscopy for catalyst characterisation: from the synchrotron to the lab	
C13	Jean-Pierre		Oudsen	UvA	Characterization of catalytic intermediates in biomimetic hydrogenase systems using X-ray Absorption Spectroscopy	
C14	Tilde		Pellegrini	RUG	Symmetric heteroaryl disubstituted alkenes as substrates for copper catalyzed addition of Grignard reagents	
C15	Maria		Ronda Lloret	UvA	PLASMA-ASSISTED DRY REFORMING OF C4H10	
C16	Vetrivel		Shanmugam	TU/e	Effect of promoters on Ni/SBA-15 catalysts for steam reforming of poly alcohol in microreactors	
C17	Thibaut		Stoll	DIFFER	WO3/BiVO4 junction as visible light photoactive material for gas phase water splitting	
C18	David		Strik	WUR	Bioelectrochemical systems for production of electricity, fuels and other chemicals	
C19	Ya-Qiong		Su	TU/e	Defect-induced Au Migration and Electron Transfer at the Au4/CeO2(111) Interface	
C20	Xiaobo		Sun	VU	Teaching Iron to Behave like Palladium: Rational Design of Iron-Based Catalysts for Cross-Coupling reactions	
C21	Yiwen		Tang	UvA	Building metal-organic frameworks from alkaline-earth nodes and pyrazine carboxylate linkers	
C22	Koen		Tijssen	RU	In-line optimization of heterogeneously catalyzed hydrogenation reactions using stripline NMR	
C23	Bas		Venderbosch	UvA	Spectroscopic characterization of the chromium-pyrrole catalytic ethene trimerization system	
C24	Kaj	van	Vliet	UvA	Bimolecular photoredox catalyzed cyclization	
C25	Gongbao		Wang	RUG	Study of the Nickel-Catalyzed Double SN2' Reaction of 1,6-Dichlorohexa-2,4-diyne	
C26	Sabry		Younes	TUD	Alcohol dehydrogenases mediate the reduction of thioesters	
C27	Wuyuan		Zhang	TUD	A 'Combinatorial Explosion' of Products through Photo-Chemo-Enzymatic Cascades	
C28	Wei		Zhang	UvA	Understanding the oxidative dehydrogenation of ethyl lactate to ethyl pyruvate over V2O5/TiO2 catalysts	
C29	Bart		Zijlstra	TU/e	Lateral interactions in Fischer-Tropsch Catalysis	

Coordination Chemistry and Homogeneous Catalysis						Tue 6 Dec/Wed 7 Dec
Poster number	First name	Prefix	Family name	Affiliation	Poster title	
CCHC01	Devin		Boom	VU	Insights in the Reactivity of a P-B Frustrated Lewis Pair Towards Azides	
CCHC02	Evi		Habraken	VU	Activation of Small Molecules using a Geminal P/B-based Frustrated Lewis Pair	
CCHC03	Flip		Holtrop	VU	Phenylene-bridged frustrated Lewis pair chemistry	
CCHC04	Ranajit		Mondol	RUG	Stable, crystalline boron complexes with mono-, di- and trianionic formazanate ligands	
CCHC05	Shaotao		Bai	UvA	Novel self-assembly macrocyclic L2M2 complex for highly regioselective hydroformylation	
CCHC06	Hans	de	Bruijn	LEI	Hydroaminomethylation with a cobalt-based catalytic system; a combined experimental and theoretical study	
CCHC07	Jianming		Chen	UU	Towards more rigid poly-N-donor-based iron oxidation catalysts	
CCHC08	Marieke		Guijt	LEI	Pd-catalyzed carbonylation of pentenoic acids as a route to bio-based $\epsilon$ -caprolactam	
CCHC09	Arnout		Hartendorp	UvA	Towards cyclizations of small peptides in @M12L24-type supramolecular spheres	
CCHC10	Joost		Kwakernaak	UU	Cobalt catalyzed hydrosilylation reactions using a non-innocent diphosphine-ketone ligand	
CCHC11	Jing		Li	UU	A new Cp-based trioxo-rhenium catalyst for deoxydehydration of diols and polyols	
CCHC12	Christina		Wegeberg	RUG	Iron Coordination and Halogen-Bonding Assisted Iodosylbenzene Activation	
CCHC13	Silvia		D'Agostini	LEI	Iron porphyrins on derivatized ITO for use in the catalytic water oxidation reaction	
CCHC14	Bas	van	Dijk	LEI	Elucidation of the Electrochemical Oxygen Reduction Reaction by a Molecular Copper Complex	
CCHC15	Gamze		Gezer	LEI	Synthesis and Characterization of [NiFe] Complexes as Biomimetic Models of Hydrogenases	
CCHC16	Konstantin		Kottrup	LEI	Molecular electrocatalysts for oxygen evolution	
CCHC17	Michiel		Langerman	LEI	Molecular copper catalysts for the electrochemical Oxygen Reduction Reaction	
CCHC18	Feng		Jiang	LEI	Structure, Spectroscopic Properties and Reactivity of Dinuclear Cobalt(II), Iron(II), and Manganese(II) Complexes Based on Disulfide Ligand: an Experimental and Theoretical Study	
CCHC19	Suzanne		Jansze	EFPL	M2L4 Type coordination cages from functional clathrochelates as metalloligands	
CCHC20	Francesca		Milocco	RUG	SPIN-CROSSOVER IN PSEUDO-TETRAHEDRAL BIS(FORMAZANATE) IRON COMPLEXES	
CCHC21	Charl		Riemersma	UU	Flexible coordination chemistry of diimine-dialcohol ligands	
CCHC22	Bin		Sun	UvA	Structure Study On A series of Novel Chiral Subcomponents self-assembled Cages	
CCHC23	Dide		Verhoeven	UU	Base Metal Complexes of a Diphosphine-Ketone and a Diphosphine-Imine Ligand: Toward New Metal-Ligand Cooperativity	
CCHC24	Sander		Wezenberg	RUG	Dynamic Control of Anion Binding Affinity and Selectivity	
CCHC25	Depeng		Zhao	RUG	Dynamic control of chirality of transition metal complex with molecular motor	

Chemistry and Structure of Materials						Tue 6 Dec/Wed 7 Dec
Poster number	First name	Prefix	Family name	Affiliation	Poster title	
CSM01	Layla		Broers	WUR	The Perfect Package	
CSM02	Esther	van	Andel	WUR	Novel sulfobetaine showing improved antifouling performance using complex biological media	
CSM03	Sjoerd		Jansma	TU/e	Hydrogen-bonded oligo(dimethylsiloxane) liquid crystals for patterning via self-assembly	
CSM04	Luuk		Kortekaas	RUG	Solvation Dependent Redox-Gated Fluorescence and Photoswitching in a Diarylethene-Based Sexithiophene Polymer Film	
CSM05	Bao		Li	TU/e	Mechanochemistry: towards new mechanisms, catalysts and switches	
CSM06	Jody		Lugger	TU/e	Nano-structured materials based on hydrogen-bonded columnar discotic liquid crystals	
CSM07	Anna		Prydatko	LEI	Robust durable superhydrophobic coatings with hierarchical surface structure	
CSM08	Hadi		Arjmandi-Tash	LEI	Thinner than graphene: Twisted nanogaps form interfacial holes	



<b>CSM09</b>	Amedeo		Bellunato	LEI	Stailized aminothiols Self-Assembly Monolayers for layer by layer deposition on gold thin films.
<b>CSM10</b>	Liuba		Belyaeva	LEI	Molecular caging of graphene with cyclohexane: a chemical platform for liquid-liquid electronics and transfer
<b>CSM11</b>	Pauline	van	Deursen	LEI	Solvent substituted hydrogels as a platform for studying Van der Waals transparency
<b>CSM12</b>	Wangyang		Fu	LEI	Fruit, flowers and vegetables can be kept longer using new graphene sensor
<b>CSM13</b>	Lin		Jiang	LEI	The electrical nature in the electrochemistry of graphene doped with sp3 and vacancy-like defects
<b>CSM14</b>	Xue		Liu	LEI	Two-Dimensional Metal-Organic Framework Single Layer Sheets with Nanopores for Sequencing
<b>CSM15</b>	Lia		Lima	LEI	Graphene-stabilized lipid monolayer heterostructures: a novel biomembrane superstructure
<b>CSM16</b>	Özgün		Attila	UU	Imaging of Carbon Deposits on H-ZSM-5 Crystals with NanoSIMS
<b>CSM17</b>	Sander		Brugman	RU	Locating the counter ions at the muscovite mica – electrolyte interface
<b>CSM18</b>	Karthikeyan		Gnanasekaran	TU/e	Quantitative electron tomography of hierarchically assembled rod-like systems
<b>CSM19</b>	Daniel		Hermida-Merino	NWO-ESRF	Science on DUBBLE at ESRF
<b>CSM20</b>	Klaartje		Houben	UU	uNMR-NL - A ultra high field NMR facility for the Netherlands
<b>CSM21</b>	Yifei		Xu	TU/e	DNA directed CaCO3 thin films
<b>CSM22</b>	Prashant		Bhaskar	TUD	Carrier mobility and recombination dynamics in 1D and 2D semiconductor nanocrystals
<b>CSM23</b>	Marco		Carlotti	RUG	Exploring Through-Space Conjugation in Molecular Junctions
<b>CSM24</b>	Silke		Diedenhofen	TUD	Liquid Exfoliation of Phosphorene
<b>CSM25</b>	Medea		Kosian	WUR	How can we create the ultimat non-stick stainless steel?
<b>CSM26</b>	Luting		Song	UvA	Template-Directed Hydrothermal Carbonization of Nitrogen-Containing Carbohydrates: A New Approach for Macroscopic-Scale Synthesis of Hetroatoms-Doped Carbon Nanofiber Aerogels
<b>CSM27</b>	Georgios		Zafeiropoulos	DIFFER	Polymeric electrolyte photoelectrochemical cell
<b>CSM28</b>	Frans		Dekker	UU	Synthesis of cubic colloids for well-defined depletion interactions
<b>CSM29</b>	Rifat		Kamarudheen	DIFFER	Plasmon-driven synthesis and assembly of hierarchical nanostructures
<b>CSM30</b>	Nicholas		Kirkwood	TUD	The influence of protic additives on the nucleation and growth of CdSe nanocrystals and magic-sized clusters
<b>CSM31</b>	Michael		Meijer	LEI	Ruthenium prodrug decoration of water dispersible upconverting nanoparticles (UCNPs) for near-infrared photo-activated chemotherapy (PACT)
<b>CSM32</b>	Giulia		Mirabello	TU/e	Magnetite synthesis through an iron phosphate precursor phase
<b>CSM33</b>	Mohammad-Amin		Moradi	TU/e	Hybrid materials based on self-assembled nano building blocks
<b>CSM34</b>	Willem		Noorduyn	AMOLF	Balancing interfacial free energy & supersaturation to direct nucleation & growth
<b>CSM35</b>	John		Pold	UU	Cation Exchange on 2-Dimensional Quantum Dot Superlattices
<b>CSM36</b>	Matteo		Parente	DIFFER	Photochemistry of metal@semiconductor core@shell nanostructures
<b>CSM37</b>	Maaike	van der	Sluijs	UU	Synthesis of luminescent CdSe nanoplatelets and self-assembly in 3D spherical supraparticles
<b>CSM38</b>	Eleanor		Townsend	RU	On additive induced creeping of sodium chloride
<b>CSM39</b>	María		Gélvez-Rueda	TUD	Charge and excited state dynamics in 2D halide perovskites
<b>CSM40</b>	Jarich		Haitjema	UvA	Organometallic tin-oxo cages used as novel photoresist materials
<b>CSM41</b>	Henrieke		Heideman	RUG	Directional Movement of Light-Driven Molecular Motors on Surfaces
<b>CSM42</b>	Eveline		Maassen	TU/e	Reversible networks for UV curable materials
<b>CSM43</b>	Xinkai		Qiu	RUG	Soft Device Fabrication Comprising Photosystem I
<b>CSM44</b>	Bruno Miguel		Rocha Martins	ARCNL	Single Nanometer Nanoparticles for Application as EUV Photoresists
<b>CSM45</b>	Rochan		Sinha	DIFFER	The Electrochemistry of High Ion Flux Helium Plasma Exposed Hematite Thin Films
<b>CSM46</b>	Bas		Salzmann	UU	Towards luminescent temperature sensing in catalytic environments using Y2O3:Eu3+/Al2O3 complexes
<b>CSM47</b>	Machi		Takeuchi	TU/e	Structure Analyses of Temperature-Sensitive Color-Change Properties of a Crystalline Organic Compound through Intercalation
<b>CSM48</b>	Langping		Tu	UvA	Energy migration upconversion dynamics in “dopant ions spatial separated” heterogeneous nanostructure
<b>CSM49</b>	Yihui		Zhao	DIFFER	Structural and Photo-electrochemical Properties of WO3 Thin Films Fabricated in Diverse Partial Pressures of Oxygen
<b>CSM50</b>	Lianjia		Wu	Other	Metal oxo-clusters as model EUV photoresists
<b>CSM51</b>	Tom		van Daal	TU/e	Mechanoluminescence; Finding new probes to elucidate polymer failure mechanisms

Design & Synthesis					Wed 7 Dec/Thu 8 Dec
Poster number	First name	Prefix	Family name	Affiliation	Poster title
<b>DS01</b>	Kelly		Ackermans	VU	Imidoylative Sonogashira Cascade towards Pharmaceutically Valuable 4-Aminoquinolines
<b>DS02</b>	Jeannine		Bathke	UMCG	Bringing β-Lactam Antibiotics Back to Life
<b>DS03</b>	Casper	de	Boer	LEI	Synthesis of Glycosidase Inhibitors and Activity Based Probes
<b>DS04</b>	John		Braun	VU	A chemoenzymatic approach towards Bullatacin
<b>DS05</b>	Wojciech		Danowski	RUG	Unidirectional rotary motion of molecular motor in the solid state
<b>DS06</b>	Verónica		Estévez Closas	VU	Fused lactone or lactam? Multicomponent reactions choose
<b>DS07</b>	Hidde		Elferink	RU	Stereoselective β-Mannosylation by Neighboring-Group Participation
<b>DS08</b>	Pieter		Gilissen	RU	Methyl ethers as masked ketones
<b>DS09</b>	Mickel		Hansen	RUG	Direct and Versatile Synthesis of Red-Shifted Azobenzenes
<b>DS10</b>	Mickey		Harvey	LEI	Synthesis and application of Schistosoma Mansoni glycans
<b>DS11</b>	Tim		Hogervorst	LEI	Exploration of crosstalk between CLRs and TLRs using single molecule vaccine modalities
<b>DS12</b>	Gydo	van der	Heijden	VU	Applications of 2-bromo-6-isocyanopyridine as novel convertible isocyanide
<b>DS13</b>	Mira		Holzheimer	RUG	Asymmetric Total Synthesis of the Mycobacterial Glycolipid DAT2
<b>DS14</b>	Roel		Klein Nijenhuis	UvA	The Formal Total Synthesis of Solanoeclipin A
<b>DS15</b>	Michael		Lerch	RUG	Investigations on the photoswitching mechanism of Donor-Acceptor Stenhouse Adducts
<b>DS16</b>	Kaizheng		Liu	RU	Synthesis of bio-functionalized polyisocyanopeptide(PIC) hydrogel for in-vitro 3D stem cell culture

DS17	Qiang		Liu	LEI	Synthesis of Ribosyl-ribosyl-adenosine trisphosphate the branched portion of poly-ADP-ribose
DS18	Mathijs		Mabesoone	TU/e	A porphyrin-based reaction network for supramolecular buffering of catalysts
DS19	Jerre		Madern	LEI	Glycosylation studies with 4-thio furanoside donors
DS20	Mikkel		Marqvorsen	LEI	Direct glycosylation with GlcNAc – New mechanistic insights
DS21	Jeanine	van	Mechelen	LEI	Synthesis of orthogonally protected bacillosamine
DS22	Rens		Mensink	RU	Participation in glycuronic acid lactone glycosylations
DS23	Pablo		Ortiz	RUG	Catalytic asymmetric alkylation of enolizable ketimines using Grignard reagents
DS24	Barry		Oppelaar	VU	Synthesis of polycyclic spiroindolines by highly diastereoselective interrupted Ugi cascade reactions
DS25	Eduardo		Palao	RU	Synthesis of Spiro[piperidine-pyridoindole] Derivatives by an Acid-Catalyzed Pictet–Splenger Reaction from alpha-arylenylamine
DS26	Krishnili		Ramratan	VU	Skeletal Diverse Synthesis of Polycyclic Heterocycles via the Sequence of Multicomponent Reaction and Intramolecular Cyclizations
DS27	Alejandra		Riesco-Dominguez	RU	Enantio- and diastereoselective synthesis of compound libraries based on the Piperidin-4-one scaffold
DS28	Diederik		Roke	RUG	A molecular motor – diarylethene switch hybrid
DS29	Jordy		Saya	VU	Unexpected Influence of Fluorinated Alcohol Solvents in an “Acidless” Passerini/Ugi-type Reaction
DS30	Sybrin		Schroder	LEI	Endo-alpha-mannosidase activity-based probe
DS31	Tjerk		Sminia	WUR	Synthesis of Novel Probes for Metabolic Oligosaccharide Engineering in Bacteria
DS32	Luuk		Stemers	UvA	
DS33	Bram		Teunissen	TU/e	Tuning reaction kinetics via supramolecular interactions
DS34	Nico		Vennik	VU	Proposed formal synthesis of enantiopure clavubicyclone using a novel Tsuji-Trost cascade cyclization
DS35	Liming		Wang	LEI	Alpha-glucans Conjugates for TB Vaccine Develepment
DS36	Yuchen		Wei	RUG	A bulky molecular motor in confined environment
DS37	Tim		Wezeman	Karlsruhe Institute of Technology	Sulfonyl Ynamides: useful tools for N-heterocyclic chemistry
DS38	Vijayendar		Yedulla	RU	Studies toward the Total Synthesis of Nahuoic acid A-E
DS39	Jielin		Zhang	RUG	Enzymatic Synthesis of Enantiopure L-Aspartic Acid Derivatives
DS40	Qingju		Zhang	LEI	Synthesis of repeating units of Zwitterionic Type 1 Capsular Polysaccharide (SP 1)

Lipids & Biomembranes					Wed 7 Dec/Thu 8 Dec
Poster number	First name	Prefix	Family name	Affiliation	Poster title
LB01	Xue		Bao	UU	Rewiring of lipid metabolism in a yeast mutant devoid of the major membrane lipid phosphatidylcholine
LB02	Amin		Abolghassemi Fakhree	UT	The number of a-synuclein proteins per vesicle gives insights into its physiological function
LB03	Rianne		Bartelds	RUG	Hydrocarbons have a small effect on phase separating giant unilamellar vesicles
LB04	Nan-Nan		Deng	RU	Microfluidic Assembly of Monodisperse Giant Vesosomes for Artificial Cell Models
LB05	Margriet		Hokken	UU	Loss of ER-mitochondria contact sites impairs transport of lipids to mitochondria in yeast overexpressing SCT1
LB06	Sabrina		Koch	RUG	Lipid-dependent SecA activity
LB07	Ruud		Korver	UvA	Halotropism re-visited: biochemical fundamentals behind changes in root growth direction during salt stress
LB08	Hetty		Manenschijn	University of Geneva	The contribution of myosin motors to membrane bending in endocytosis
LB09	Mike		Renne	UU	Regulation of membrane fluidity in S. cerevisiae
LB10	Jeroen		Strating	UU	Viral hijacking of host cell membrane contact site machinery
LB11	Remco		Rodenburg	UU	Unraveling the membrane protein palmitoylation signal
LB12	Lukasz		Syga	RUG	Slow diffusion, steric exclusion and targeted protein delivery determine the localization of plasma membrane transporters
LB13	Mark		Verheijden	UT	A cell interface with tuneable dynamics using lipidated peptides
LB14	Keni		Yang	RUG	The Role of Nanoparticle Corona on Liposome-Cell Interactions
LB15	Jing (Nicola)		Yang	LEI	Application of Coiled Coil Peptides in Liposomal Anti-Cancer Drug Delivery Using a Zebrafish Xenograft Model

Medicinal Chemistry					Wed 7 Dec/Thu 8 Dec
Poster number	First name	Prefix	Family name	Affiliation	Poster title
MC01	Eman		Abdelraheem	RUG	TOWARD LIBRARIES OF ARTIFICIAL MACROCYCLES
MC02	Sebastian		Andrei	TU/e	Towards a selective stabilizer of the 14-3-3/Notch4 protein protein interaction
MC03	Janez Zan		Bulc	VUMC	Carbon-11 Labeled Substance P1-7 Peptidomimetics as Imaging Agents for the Treatment of Neuropatic Pain
MC04	Antoni		Blaazer	VU	Fragment-Based Screening in Tandem with Phenotypic Screening Provide Novel Antiparasitic Hits
MC05	Anja		Busemann	LEI	Preparation of alkyne-modified ruthenium complexes for pull down experiments
MC06	Jordi Amat		Cuello-Garibo	LEI	Photoreactivity and phototoxicity of a series of strained ruthenium-based complexes with N,S-coordinating ligands
MC07	Hui		Deng	LEI	Design and Enantioselective Synthesis of Chemical Probes to Study Brain Lipid Signaling
MC08	Marc	van	Dijk	VU	Comprehensive and automated Linear Interaction Energy based binding-affinity prediction Applied to Cytochrome P450 aromatase inhibitors
MC09	Annelot	van	Esbroeck	LEI	BIA 10-2474 disrupts lipid metabolism and glutamatergic signaling in human neurons

MC10	Xavier		Gómez-Santacana	VU	PHOTOISOMERIZABLE PHENYLAZOPYRIDINES ENABLE THE CONTROL OF METABOTROPIC GLUTAMATE RECEPTOR SUBTPE 5 ACTIVITY WITH LIGHT
MC11	Sebastian		Grimm	LEI	Hit identification strategy to overcome drug-induced FLT3-kinase inhibitor resistance
MC12	Hao		Guo	RUG	Is photo-activation a novel mechanism for pan assay interference compounds (PAINS)?
MC13	Kamaleddin		Hajmohammad-ebrahimtehrani	UU	Small molecule inhibitors of bacterial metallo-β-lactamases: Synergy assays and Zinc-binding studies
MC14	Ingrid	't	Hart	UU	Chemoenzymatic synthesis of Disialosyl Globopentaosylceramide (DSGb5) for cancer treatment
MC15	Alwin		Hartman	RUG	Structure-Based Optimisation of Inhibitors of the Aspartic Protease Endothiapepsin
MC16	Raimond		Heukers	VU	Nanobody-mediated modulation of oncogenic properties of HCMV-encoded chemokine receptor US28
MC17	Erik	de	Heuvel	VU	Design of novel TbrPDEB1/B2 inhibitors for the treatment of human African trypanosomiasis
MC18	Mark		Hoorens	UMCG	Hemithioindigo photoswitches for biological applications
MC19	Miranda		Jekhmane	UU	Rational design of a self-assembling peptide for the delivery of nucleic acids
MC20	Ming		Jiang	LEI	Design, Synthesis and Activity Assay of Highly Selective, Potent and Drug-like DAGL-α Inhibitor
MC21	Varsha		Jumde	RUG	Design and Synthesis of Bioisosteres of Acylhydrazones as Stable Inhibitors of the Aspartic Protease Endothiapepsin
MC22	L.H.J.		Kleijn	UU	Total synthesis of the calcium-dependent lipopeptide antibiotic Laspartomycin C and investigations into its antibacterial mode of action
MC23	Danny		Lenstra	RU	Development of highly active inhibitors of SETD7 histone lysine methyltransferase
MC24	Kai		Liu	TUD	Investigation of protection effect of different coating layers on irradiated Ho2(CO3)3 nanoparticles
MC25	Elma		Mons	LUMC	Modification of the Electrophile in Ubiquitin-based Probes towards Labeling of Specific DUBs
MC26	Elliot		Mock	LEI	Mapping NAPE lipid signaling using photoaffinity labeling coupled with chemoproteomics
MC27	Anna		Pees	VU	Development of high specific activity [18F]trifluoromethylation methods for PET tracer synthesis
MC28	Friederike		Reeßing	UMCG	Synthesis of light-responsive MRI contrast agents
MC29	Alen		Sevšek	UU	Bicyclic isoureas derived from 1-deoxynojirimycin are potent inhibitors of β-glucocerebrosidase
MC30	Eline		Sijbesma	TU/e	Fragment-based drug discovery to stabilize protein-protein interactions
MC31	Maarten		Sijm	VU	Human PDE4 inhibitor analogues with submicromolar activity against Trypanosoma cruzi
MC32	Kaja		Sitkowska	RUG	Photoactivated Chemotherapy
MC33	Inna		Slynko	VU	Elucidation of the Structural Determinants of Functional Activity Switches between Histamine H3 Receptor Orthologues
MC34	Marjolein		Soethoudt	LEI	Conformation-dependent labeling of the cannabinoid CB2 receptor for proof of target engagement in live cells
MC35	Dieuwertje		Streefkerk	UvA	Scaffold-assisted Synthesis of Multicyclic Peptides via Orthogonal Ligation Strategies
MC36	Wiktor		Szymanski	UMCG	Light-Controlled Histone Deacetylase (HDAC) Inhibitors: Towards Photopharmacological Chemotherapy
MC37	Abbas	Al	Temimi	RU	Is the Length of Lysines Side Chains Optimal for Histone Lysine Methyltransferase Catalysis?
MC38	Stephanie		Thee	VU	Analysis of Fragment Stabilizers of 14-3-3/ERα Interaction
MC39	Thea		van den Bosch	RUG	Lysine deacetylase inhibitors as potential drugs in inflammatory diseases
MC40	Gábor		Wágner	VU	Covalent targeting of the histamine H3 receptor
MC41	Zhiyong		Wang	VU	Rupatadine analogs to investigate binding kinetics on the histamine H1 receptor
MC42	Hannah		Wapenaar	RUG	Challenges in targeting histone acetyltransferases: A KAT8 case story
MC43	Tom	van der	Wel	LEI	A Chemical Genetics Approach towards Subtype-selective Inhibition of Diacylglycerol Lipases
MC44	Juan		Zhou	LEI	Discovery and application of an activity-based probe for N-acyltransferases

Macromolecules						Tue 6 Dec/Wed 7 Dec
Poster number	First name	Prefix	Family name	Affiliation	Poster title	
MM01	Anna		Abbadessa	UU	Glycosaminoglycan-based Microgels for Controlled Release of Proteins from Hydrogel Scaffolds	
MM02	Beatrice	B	Adelizzi	TU/e	Towards sequence controlled supramolecular copolymerization	
MM03	Maarten		Danial	CSIRO Australia	Polymers with activity against HIV	
MM04	Sjaak		Jong	UU	Quantitative 13C- NMR for fast urea concentration determination in complex mixtures	
MM05	Marko		Mihajlovic	TU/e	High-toughness supramolecular hydrogel based on hydrophobic interactions	
MM06	Marzieh		Najafi	UU	Core crosslinking of flower like micelles using native chemical ligation	
MM07	Tim		Paffen	TU/e	Improved supramolecular buffering; multivalency in ring-chain systems	
MM08	Huey Wen		Ooi	UM	Towards development of synthetic dynamic bioinks for 3D printing	
MM09	Joe		Patterson	TU/e	Watching block copolymer self-assembly with liquid phase electron microscopy	
MM10	Victorio		Saez Talens	LEI	Modulating hydrogen bond strength in squaramide-based supramolecular polymers	
MM11	Daniël		Schoenmakers	RU	Biomimetic networks of crosslinked polyisocyanide hydrogels	
MM12	Marcin		Sleczkowski	TU/e	A versatile strategy for position-controlled functional polydimethylsiloxane	
MM13	Nathan	Van	Zee	TU/e	Pathway complexity in the self-assembly of biphenyl tetracarboxamides in organic solvents	
MM14	Masyitha		Ambarwati	RUG	Enzymatic Polymerization of Telechelic and Three-Arm PTHF-b-Amylose	
MM15	Lies		Fliervoet	UU	HETERO-FUNCTIONAL PEG MACROINITIATOR FOR SYNTHESIS OF ABC TRIBLOCK COPOLYMERS	
MM16	Csaba		Fodor	RUG	Biocatalysis in high-value bio-plastic production from lignin derived biomass	
MM17	Dina		Maniar	RUG	Enzymatic Synthesis of Furan 2,5-Dicarboxylic Acid Based Heteroatom Polyamides	
MM18	Jose Augusto		Berrocal	TU/e	Nano-patterned self-assembly of monodisperse naphthalenediimide-oligodimethylsiloxane plastic crystals	
MM19	Bas	van	Genabeek	TU/e	Dispersity and Tacticity Effects in Ultra-Defined Block Copolymers	
MM20	Zino		Leijten	TU/e	Measuring stability of polymer nanocomposites in (Cryo)TEM	
MM21	Niels		Meereboer	RUG	Confinement effect on the Curie transition in ferroelectric block copolymers	
MM22	Dirk Jan		Mulder	TU/e	Nanoporous Polymer Materials based on Liquid Crystalline Networks	
MM23	Jeffrey		Murphy	TU/e		
MM24	Ivan		Terzic	RUG	Self assembly of P(VDF-co-TrFE) based block copolymers	
MM25	María Paula		Vena	TU/e	Formation and mineralization of nanoparticles with bicontinuous internal structure	
MM26	Jin		Xu	RUG	Polymer-templated multiferroic nanocomposites	
MM27	Paula		de Almeida	RU	Strain-stiffening behaviour in PIC-ELR hybrid systems: Their potential as stimuli responsive scaffolds	
MM28	Alexei		Filippov	WUR	Thermoresponsive anionic ABA triblock copolymers for nanostructured adhesive complex coacervates	
MM29	Digvijay		Gahtory	WUR	Exploring dynamic interactions on surfaces	
MM30	He		Huang	UT	Host-guest chemistry of fluorinated azobenzene to build up dynamic systems	
MM31	Hitesh		Khandelwal	TU/e	Smart Windows Based on Cholesteric Liquid Crystal Polymer	
MM32	Bryn		Monnery	Ghent University	Thermoresponsive ABA Triblock Poly(2-oxazoline)s as Potential Injectable Hydrogels	
MM33	Stijn		Kragt	TU/e	Temperature-responsive coatings based on reactive mesogens and liquid crystalline polymers	
MM34	Roel	van	Raak	TU/e	Sunlight responsive liquid crystal actuators	
MM35	Esther		Roeven	WUR	New approaches towards zwitterionic antifouling coatings	
MM36	Ghislaine		Vantomme	TU/e	Light induced self-oscillation of hydrazone-based liquid-crystal networks	

<b>MM37</b>	Yunlong		Yu	UT	Specific Anion Effects on the Hydration and Tribological properties of Zwitterionic PMPC Brushes
<b>MM38</b>	Kaihuan		Zhang	UT	Redox-active poly(ferrocenylsilane)s as responsive materials
<b>MM39</b>	Hongbo		Yuan	RU	Hydrogen Bonds Controlled Tripeptide-Derived Polyisocyanides Hydrogels with High Gelation Temperatur
<b>MM40</b>	Ilse	van	Hees	WUR	The polymerization of PNIPAM-b-PDMAEMA-b-PNIPAM using difunctional RAFT-agents

Nucleic Acids						Wed 7 Dec/Thu 8 Dec
Poster number	First name	Prefix	Family name	Affiliation	Poster title	
<b>NA01</b>	Merel		Derksen	RU	Identification of human RNase MRP/P substrates	
<b>NA02</b>	Clara	van	Emmerik	LEI	Nucleosomal DNA labeling for interaction studies by NMR	
<b>NA03</b>	Roman		Koning	LUMC	Asymmetric cryo-EM reconstruction of phage MS2  reveals genome structure in situ	
<b>NA04</b>	Joyce		Lebbink	EMC	Molecular mechanism of daughter strand incision during DNA mismatch repair	
<b>NA05</b>	Clemens		Mayer	RUG	An epigenetics-inspired DNA-based data storage system	
<b>NA06</b>	Fatema Zahra		Rashid	LEI	The 3-dimensional organization of the bacterial genome and its interplay with gene expression	
<b>NA07</b>	Martijn		Zwinderman	RUG	What Happens to Nucleosomes during Chromatin Replication?	

Protein Research						Wed 7 Dec/Thu 8 Dec
Poster number	First name	Prefix	Family name	Affiliation	Poster title	
<b>PR01</b>	Ingy		Abdallah	RUG	Amorphadiene Synthase: A Step Forward in Unraveling the Enigma of its Catalytic Mechanism	
<b>PR02</b>	Daan		Geerke	VU	Enhancing protein-drug binding prediction	
<b>PR03</b>	Anniek	den	Hamer	TU/e	Small Molecule-Induced Enzyme Activation on 14-3-3 Scaffolds	
<b>PR04</b>	Panagiotis		Koukos	UU	SpotOn: A web server for the prediction of protein-protein binding hotspots	
<b>PR05</b>	Rosa		Luirink	VU	Binding Pose and Affinity Prediction for Engineered Cytochrome P450 Mutants	
<b>PR06</b>	Siddarth		Narasimhan	UU	EGFR dynamics change during activation in native membranes as revealed by NMR	
<b>PR07</b>	Elvira		Romero	RUG	Characterization and Crystal Structure of a Robust Cyclohexanone Monooxygenase	
<b>PR08</b>	Revina	van	Scherpenzeel	UU	Towards structural studies of Wnt signaling	
<b>PR09</b>	Deniz		Ugurlar	UU	Assembly of complement C1 is dynamic	
<b>PR10</b>	Yizhou		Wang	RUG	Creation of antagonists for the RANK-RANKL pathway by modulating the DE-loop	
<b>PR11</b>	Magdalena		Wójcik	RUG	Directed evolution of sortase A from Streptococcus pyogenes	
<b>PR12</b>	Ramon	van den	Bos	UU	Structural studies of the alternative pathway of Complement	
<b>PR13</b>	Patricia		Alvarez Sieiro	RUG	Formation of heterodimeric OpuA for smFRET studies	
<b>PR14</b>	Cecilia		de Agrela Pinto	UU	Probing the structure of the 200 kDa B-barrel assembly machinery complex in liposomes	
<b>PR15</b>	Srividya		Ganapathy	LEI	Towards the adaptation of rhodopsin proton-pumps	
<b>PR16</b>	Alisa		Garaeva	RUG	Structural and biochemical characterization of human amino acid transporter ASCT2	
<b>PR17</b>	Ryan		Henderson	RUG	Understanding the proton translocation pathway of the yeast maltose permease	
<b>PR18</b>	Joury	van 't	Klooster	RUG	Asymmetry in inward- and outward-affinity constant of transport explain unidirectional lysine flux in Saccharomyces cerevisiae	
<b>PR19</b>	Jelger		Lijcklama a Nijeholt	RUG	The substrate binding domain of GlnPQ docks on the channel in the closed state and initiates the ATP cycle.	
<b>PR20</b>	Marjolein		Mijnders	UU	Cellular Protein Chemistry, Bijvoet Center for Biomolecular Research, Faculty of Science, Utrecht University	
<b>PR21</b>	Wout		Oosterheert	UU	Expression and purification of a human six-helical transmembrane protein family	
<b>PR22</b>	Stephan		Rempel	RUG	A new vitamin B12 transporter, BtuM	
<b>PR23</b>	Gea		Schuurman-Wolters	RUG	On the relationship between effective receptor and transport in the GlnPQ ABC importer	
<b>PR24</b>	Hendrik		Sikkema	RUG	Elucidating the transport mechanism of the ABC-transporter OpuA: towards smFRET studies on OpuA in monodisperse nanoparticles	
<b>PR25</b>	Weronika		Stanek	RUG	Biochemical characterization of transport in the ECF transporters	
<b>PR26</b>	Rajkumar		Singh	RUG	Biochemical and Structural characterization of NadR from L.Lactis in substrate bound and free conformation	
<b>PR27</b>	Artem		Stetsenko	RUG	First glance at zinc membrane transporter ZntB	
<b>PR28</b>	Lotteke		Swier	RUG	Insight in the transport mechanism of ECF transporters by crystal structures	
<b>PR29</b>	Laura		Tadè	UU	CFTR Folding and Function from the Endoplasmic Reticulum to the Plasma Membrane	
<b>PR30</b>	Gianluca		Trinco	RUG	Biochemical characterization of GltTk	
<b>PR31</b>	Hedwich		Vlieg	UU	Structural studies of neuronal growth inhibition	
<b>PR32</b>	Soumya	Deep	Chatterjee	LEI	A 15N CPMG relaxation dispersion experiment optimized for high fields and broad bandwidth.	
<b>PR33</b>	Cunliang		Geng	UU	Exploring the interplay between experimental methods and the performance of predictors of binding affinity change upon mutations in protein complexes	
<b>PR34</b>	Deni		Mance	UU	Novel high-sensitivity approaches for in-situ NMR	
<b>PR35</b>	Igor		Nederlof	LEI	New Timepix Detector enables Single Crystal Structure Determination of Beam Sensitive Nano-Crystals	
<b>PR36</b>	Viviana		Neviani	UU	A novel double tag system for efficient purification of tetraspanins	
<b>PR37</b>	Maarten		Tuijtel	LEI	Correlative super resolution cryo Light and Electron Microscopy	
<b>PR38</b>	Enrico		Zurlo	LEI	Rigid spin labels for improved distance and dynamics measurements in protein and peptides	
<b>PR39</b>	Baojie		Zhang	RUG	DR5 fucosylation enhances sensitivity to TRAIL in colon cancer cells	
<b>PR40</b>	Ivan		Corbeski	UU	Interaction of a histone chaperone involved in DNA repair with a core histone complex	
<b>PR41</b>	Xin		Chen	RUG	Investigating the peroxisomal membrane associated degradation (PMAD) pathway in yeast	
<b>PR42</b>	Emanuela		Crisafi	LEI	Investigating lipid interactions that control the molecular switch in photosynthetic light harvesting complex	
<b>PR43</b>	Wouter		Elings	LEI	Phosphate catalyses the recovery of Mycobacterium tuberculosis β-lactamase from clavulanic acid inhibition	
<b>PR44</b>	Emilia		Grad	RU	Coiled coils as tunable and mechanosensitive mechanical elements.	
<b>PR45</b>	Maithili		Krishnan	LEI	PsbS : a plant pH sensor regulating Photosynthesis	
<b>PR46</b>	Boqun		Liu	RUG	A comparison of control over crowding-induced protein compression in the cell versus in vitro.	
<b>PR47</b>	Jonas		Noguera Lopez	TUD	Cell- Free Expression and Functional Reconstitution of E. coli Division Proteins	
<b>PR48</b>	Simone		Wouters	TU/e	DNA-based control of antibody activity	
<b>PR49</b>	Tjeerd		Pols	RUG	Building a Synthetic Cell: Long-term metabolic energy generation inside lipid vesicles	
<b>PR50</b>	Doreth		Kok	NKI	DNA Mismatch repair – studying the activation states with cryo-EM	
<b>PR51</b>	Tao Ju		Cui	TUD	Argonaute target search is facilitated by long distance diffusion	
<b>PR52</b>	Yoshitaka		Hiruma	NKI	Characterization of Mps1 kinase by NMR spectroscopy	
<b>PR53</b>	Heyi		Zhang	LEI	Reduced electrostatic repulsion stabilizes histone H2A.Bbd-H2B dimer	
<b>PR54</b>	Tania		Moran Luengo	UU	Hsp90 releases the break on the Hsp70 folding path	
<b>PR55</b>	Luca		Ferrari	UU	Molecular chaperones stabilise protein oligomers linked to neurodegeneration	
<b>PR56</b>	Magdalena		Wawrzyniuk	UU	Disordered proteins in the eyes of a molecular chaperone.	
<b>PR57</b>	Marcel	van	Willigen	UU	A late assembly step can disrupt a well-folded domain in proteins	
<b>PR58</b>	Nadia		Leloup	UU		
<b>PR59</b>	Yanzhang		Luo	UU	Probing minus-end targeting proteins in complex with microtubules by solid-state NMR	
<b>PR60</b>	Dimphna		Meijer	UU	Cell-adhesion molecule dimerization during synapse formation (max 300 words)	



PR61	Sandra		Ortega Ugalde	VU	Ability of endo- and exogenous redox-partners to reduce and support the catalytic activity of Mycobacterium tuberculosis Cytochrome P450 enzymes
PR62	Matti		Pronker	UU	Structural basis of the myelin-axon interaction
PR63	Susanne		Terheyden	RUG	Biochemical and Structural analyses of Roco proteins to study LRRK2-mediated Parkinson disease
PR64	Dragana		Vidovic	UU	Dissecting the role of molecular chaperones in co-translational folding of membrane proteins
PR65	Hui Ying		Yeoh	UU	Mechanisms of the folding of second nucleotide binding domain of CFTR

Process Technology					Wed 7 Dec/Thu 8 Dec
Poster number	First name	Prefix	Family name	Affiliation	Poster title
PT01	Liangliang		Lin	TU/e	An atmospheric pressure microplasma process for nanoparticle synthesis and their bio-application study
PT02	Marc		Escriba Gelonch	TU/e	Process intensification for Vitamin D3: Continuous laser-based photo high-T process with integrated continuous anti-solvent crystallization
PT03	Dannie	van	Osch	TU/e	Removal of alkali and transition metal ions from water with hydrophobic deep eutectic solvents
PT04	Yung		Ngothai	TU/e	Sustainability Assessment of Intensified, Integrated Laser-based Photo Micro-Flow Process to Manufacture Vitamin D3
PT05	Natan	J. W.	Straathof	TU/e	Accelerated Photoredox Catalysis in Continuous Microflow
PT06	Vittorio		Saggiomo	WUR	Complex microfluidic devices by Embedded SCAffold RemovinG Open Technology: ESCARGOT

Soft Matter					Wed 7 Dec/Thu 8 Dec
Poster number	First name	Prefix	Family name	Affiliation	Poster title
SM01	Frankje	de	Boer	UU	Bio-based Colloidal Colorants
SM02	Fuqiang		Chang	UU	Structure formation of colloidal dumbbells at oil-water interfaces
SM03	Dennis	van	Eldik	UU	Self-propelling Superballs
SM04	Carla		Fernández Rico	UU	Synthesis of photo-crosslinkable surface modified polystyrene particles
SM05	Ellen		Heuven	UU	Encapsulation of micron-sized large colloids by oppositely charged anisotropic snowman particles
SM06	Jan Bart	ten	Hove	WUR	Monodisperse, water-soluble gold nanoparticles for biosensing applications
SM07	Olessya		Loiko	TU/e	Charged co-oligomers: route towards polymer-Gibbsite nanocomposites
SM08	Sebastian		Rzadkiewicz	TU/e	Self-assembly of nanoparticles into colloidal crystals
SM09	Serhii		Mytnyk	TUD	Microcapsules with a permeable hydrogel shell continuously produced by all-aqueous microfluidics
SM10	Edyta		Swider	RUMC	Rational design of PLGA-perfluorocarbon nanoparticles for biomedical applications
SM11	Shuaiqi		Guo	TU/e	Structural insights into preventing the biofilm formation of bacteria
SM12	Pim		Frederix	RUG	Studying self-assembling bionanostructures using computational techniques
SM13	Yuliia		Vyborna	Other	DNA-grafted supramolecular polymers: synthesis, self-assembly and potential applications
SM14	Melissa		Rinaldin	LEI	Phase separation patterns in artificial lipid membranes: the role of geometry and composition
SM15	Tjalling		Canrinus	RUG	Real time imaging of fibre growth during gel formation
SM16	Vasudevan		Lakshminarayanan	TUD	pH driven microstructural differences in an acid triggered supramolecular gel
SM17	Matija		Lovrak	TUD	Supramolecular Hydrogel Freestanding Objects Made Using Reaction-Diffusion
SM18	Ivan		Rehor	UU	Multifunctional microparticles for labelling food and pharmaceutical products
SM19	Anne		Weijkamp	UU	Tuning the elasticity of PEGDA micro particles
SM20	Hailong		Che	TU/e	Bio-inspired Multicomponent Self-assembly of Hydrogelators and Polymer Nano-objects
SM21	Jinling		Cheng	RUG	Bidirectional Photomodulation of Surface Tension in Langmuir Films
SM22	Ilias		Patmanidis	RUG	Solving the atomistic structure of supramolecular dye nanotubes
SM23	Susan	van	Rossum	TUD	Catalytic control over transient materials
SM24	Filippo		Tosi	RUG	BINOL-based self-assembled Nanotubes
SM25	Yingfeng		Tu	RU	Stimuli-Responsive Polymeric Nanomotor for movement control and drug delivery
SM26	Hanglong		Wu	TU/e	Low dose liquid phase imaging of soft matter
SM27	Stefanie		Lange	WUR	Efficient and Tunable 3D Functionalization of Fully Zwitterionic Antifouling Surface Coatings
SM28	Mark	van	Rijt	TU/e	Self-Assembly of Sequence Define Block Copolypeptides
SM29	Olga		Koshkina	RU	Perfluorocarbon-loaded polymeric nanoparticles with unusual structure for clinical and in vivo imaging
SM30	Lione		Willems	WUR	Self-assembly of artificial viruses

Structure & Reactivity					Wed 7 Dec/Thu 8 Dec
Poster number	First name	Prefix	Family name	Affiliation	Poster title
SR01	shuqin		Cao	UT	Virus Cage as Simple Template to Study the Host-guest chemisty
SR02	Daniele		Di Iorio	UT	Understanding the multivalent interactions of the Influenza Virus
SR03	Thomas		Hansen	LEI	Pyranosyl Oxocarbenium Ion Stability and Stereoselectivity
SR04	Pramod Patil		Kunturu	UT	Sunlight as a Fuel
SR05	Andrea		Leoncini	UT	Influence of chirality, pre-organization and ionic liquids on the extraction of rare earths
SR06	Xiao		Meng	TU/e	New candidates of organic ferroelectric materials
SR07	Jacopo		Movilli	UT	Engineering Monolayers For Ultrasensitive DNA Detection
SR08	Kathleen		Stout	RU	Threading Polymers through Covalently Linked Double Porphyrin Cavities
SR09	Cansel		Temiz	TUD	Optimizing Charge And Excited State Transport In Discotic Materials
SR11	Stefan	van der	Vorm	LEI	The Influence of Acceptor Nucleophilicity on the Glycosylation Reaction Mechanism
SR12	Hans		Wienk	UU	iNEXT – Infrastructure for NMR, EM and X-rays for Translational Research



Poster number	First name	Prefix	Family name	Affiliation	Poster title
ST01	Sjors		Bakels	RU	Beta-Sheet Forming Peptides probed by far-IR Action Spectroscopy
ST02	Karin	de	Groot	UvA	In silico screening protocol to identify candidate salt sensor proteins.
ST03	Ioana		Ilie	UT	From all-atom to coarse-grain simulations of alpha-synuclein
ST04	Ambiuj		Tiwari	UvA	Reacave trajectories of the Ru2+/3+ self-exchange reactions Using TPS and the connection to Marcus' theory
ST05	Francesco		Zaccaria	VU	RNA vs DNA G-Quadruplex: the origin of increased stability
ST06	Annemarie		Huijser	UT	Shedding light on dark excited states in a H2 forming photocatalyst by ps x-ray spectroscopy
ST07	Merijn		Blaakmeer	RU	Understanding the Role of Aluminium Alkyls in Ziegler-Natta Catalysts
ST08	Sridevi		Krishnamurthi	UT	Edge states in MoS2 photocatalysts
ST09	Anna		Bondarenko	RUG	Excitation energy transfer in multichromophoric systems
ST10	Stephanie	ten	Brinck	VU	The Electronic Structure of Cesium Lead Halide Perovskite Nanocrystals
ST11	Monika		Dash	UT	Exciting the building blocks of organic solar cells
ST12	Riande		Dekker	UU	Delayed emission of InP/ZnS core-shell quantum dots
ST13	Marwa		Farag	RUG	Probing the Interstate Coupling near a Conical Intersection by Optical Spectroscopy
ST14	Andres		Gregorio Puig	UU	Temperature dependence of luminescence properties on lanthanide-doped LaPO4 nanocrystals
ST15	Damla		Inan	TUD	The Effect of Solvent Polarity on the Photophysics of Artificial Light Harvesting Antenna Systems
ST16	Maria		Izquierdo	RUG	THE DISCRETE REACTION FIELD MODEL FOR LARGE SCALE MODELING OF ORGANIC PHOTOVOLTAICS
ST17	Mark		Koenis	UvA	VCDtools: a user-friendly program for analysing VCD spectra
ST18	Aditya		Kulkarni	TUD	Step-like carrier multiplication in percolative network of atomically bonded PbSe quantum dots
ST19	Tenzin		Kunsel	RUG	Structural modeling and single-aggregate spectroscopy of zinc chlorin nanotubes
ST20	Selim		Sami	RUG	Computation of dielectric constants of fullerene derivatives for organic photovoltaics
ST21	Ayush		Narsaria	VU	Rational design of near-infrared absorbing organic dye molecules
ST22	Salvatore		Cosseddu	VU	Theoretical Investigation of Dynamics at the Surface of Semiconductor Nanocrystals
ST23	Katherina		Doblhoff-Dier	LEI	Barrier heights for the H2 dissociation on Cu(111) from quantum Monte Carlo calculations
ST24	Gernot		Fuechsel	LEI	The Enigmatic HCl + Au(111) Reaction: A Puzzle for Theory and Experiment
ST25	Francesco		Nattino	LEI	Quantitative modeling of a polyatomic molecule-metal surface reaction
ST26	Jurn		Heinen	UvA	Predicting Multicomponent Adsorption Isotherms in Open-Metal Site Materials using Density Functional Theory Derived Force Field Calculations
ST27	Elham		Nour Ghassemi	LEI	Dynamics study on dissociative chemisorption of H 2 on Pt(111)
ST28	Sayan		Seal	LEI	The water-Pt(111) interface studied by path integral molecular dynamics
ST29	Khosrow		Shakouri	LEI	A high-dimensional neural network potential for the reaction of nitrogen molecules with Ru(0001)
ST30	Kirstin		Doney	LEI	High Resolution Infrared Spectroscopy of Astronomical Molecules
ST31	Sander		Lemmens	RU	Studying stardust: Spectroscopy on PAHs
ST32	Sandra		Wiersma	UvA	Gas-phase infrared spectra of astronomical Polycyclic Aromatic Hydrocarbons measured with FELICE, the Free Electron Laser for Intra-Cavity Experiments
ST33	Wim		Roeterdink	UvA	IR and fluorescence spectroscopy of astronomical PAHs
ST34	Satesh		Gangarapu	VU	Automation of Transition State Search with Qmworks
ST35	Sara		Giarrusso	VU	Insight into the decomposition of the XC potential in the physical and in the strong-coupling limit cases
ST36	Klaas		Giesbertz	VU	Approximate energy functionals for one-body reduced density matrix functional theory from many-body perturbation theory
ST37	Juri		Grossi	VU	Effect of spin statistics in the strongly correlated limit of DFT
ST38	Benjamin		Helmich-Paris	VU	Multi-reference methods in the atomic-orbital basis for extended molecular systems
ST39	Felipe		Zapata	VU	Workflows automation in quantum chemistry
ST40	Gianluca		Grimaldi	TUD	Charge transfer in composite PbSe-CdSe NC films
ST41	Gabriele		Panarelli	LEI	Towards Temperature-Cycle EPR: Chemical kinetics.
ST42	Dina		Petrova	UvA	Microscopic visualisation of contacts and friction
ST43	Xueqing		Zhang	DIFFER	Water Oxidation at Hematite Surfaces: A Theoretical Study

## Overview of Poster Pitches CHAINS 2016

**Tuesday 6 December, 12.15 - 12.25**

### room 55-57

1. Rohit Chaudhary (TU/e) - CO<sub>2</sub>-neutral Methanol Synthesis from CO<sub>2</sub> and H<sub>2</sub> by Smart-Scaled, Reaction Integrated Plasma Process - Poster C01
2. Nazila Masoud (UU) - The stability of Au and Au-Ag catalysts for the model hydrogenation and oxidation reactions - Poster C11

### Boszaal

1. Suzanne Jansze (EFPL) - M2L4 Type coordination cages from functional clathrochelates as metalloligands - Poster CCHC19

### room 58

1. Nathan Straathof (TU/e) - Accelerated Photoredox Catalysis in Continuous Microflow - Poster PT05
2. Liang Lin (TU/e) - An atmospheric pressure microplasma process for nanoparticle synthesis and their bio-application study - Poster PT01
3. Maria Ronda Lloret (UvA) - PLASMA-ASSISTED DRY REFORMING OF C<sub>4</sub>H<sub>10</sub> - Poster C15

### Parkzaal

1. Serhii Mytnyk (TUD) - Microcapsules with a permeable hydrogel shell continuously produced by all-aqueous microfluidics - Poster SM09
2. Olessya Loiko (TU/e) - Charged co-oligomers: route towards polymer-Gibbsite nanocomposites - Poster SM07
3. Frankje de Boer (UU) - Bio-based Colloidal Colorants - Poster SM01

### Auditorium

1. Digvijay Gahtory (WUR) - Exploring dynamic interactions on surfaces - Poster MM29
2. Stijn Kragt (TU/e) - Temperature-responsive coatings based on reactive mesogens and liquid crystalline polymers - Poster MM33
3. Hongbo Yuan (RU) - Hydrogen Bonds Controlled Tripeptide-Derived Polyisocyanides Hydrogels with High Gelation Temperature - Poster MM39

### Room 80/81

1. Rochan Sinha (DIFFER) - The Electrochemistry of High Ion Flux Helium Plasma Exposed Hematite Thin Films - Poster CSM45
2. Maria Gélvez-Rueda (TUD) - Charge and excited state dynamics in 2D halide perovskites - Poster CSM39
3. Yihui Zhao (DIFFER) - Structural and Photo-electrochemical Properties of WO<sub>3</sub> Thin Films Fabricated in Diverse Partial Pressures of Oxygen - Poster CSM49

### Room 63/65

1. Felipe Zapata (VU) - Workflows automation in quantum chemistry - Poster ST39
2. Marwa Farag (RUG) - Probing the Interstate Coupling near a Conical Intersection by Optical Spectroscopy - Poster ST13
3. Mark Koenis (UvA) - VCDtools: a user-friendly program for analysing VCD spectra - Poster ST17

### Room 65

1. Damla Inan (TUD) - The Effect of Solvent Polarity on the Photophysics of Artificial Light Harvesting Antenna Systems - Poster ST15
2. Merijn Blaakmeer (RU) - Understanding the Role of Aluminium Alkyls in Ziegler-Natta Catalysts - Poster ST07
3. Xueqing Zhang (DIFFER) - Water Oxidation at Hematite Surfaces: A Theoretical Study - Poster ST43

## Tuesday 6 December

**18.35 - 18.45**

### room 55-57

1. Tilde Pellegrini (RUG) - Symmetric heteroaryl disubstituted alkenes as substrates for copper catalyzed addition of Grignard reagents - Poster C14
2. Andrea George (UvA) - Designing chiral metal organic framework for enantioselective catalysis - Poster C08

### Boszaal

**No pitches**

### room 58

**No Pitches**

### Parkzaal

1. Pim Frederix - Studying self-assembling bionanostructures using computational techniques - Poster SM12
2. Mark van Rijt - Self-Assembly of Sequence Define Block Copolypeptides - Poster SM28
3. Vasudevan Lakshminarayanan (TUD) - pH driven microstructural differences in an acid triggered supramolecular gel - Poster SM16

### Auditorium

1. Beatrice Adelizzi (TU/e) - Towards sequence controlled supramolecular copolymerization - Poster MM02
2. Huey Wen Ooi (UM) - Towards development of synthetic dynamic bioinks for 3D printing - Poster MM08
3. Zino Leijten (TU/e) - Measuring stability of polymer nanocomposites in (Cryo)TEM - Poster MM20

### Room 82/83

1. Ester van Andel (WUR) - Novel sulfo betaine showing improved antifouling performance using complex biological media - Poster CSM02
2. Xue Liu (LEI) - Two-Dimensional Metal-Organic Framework Single Layer Sheets with Nanopores for Sequencing - Poster CSM14
3. Jody Lugger (TU/e) - Nano-structured materials based on hydrogen-bonded columnar discotic liquid crystals - Poster CSM06

### Room 80/81

1. Giulia Mirabello (TU/e) - Magnetite synthesis through an iron phosphate precursor phase - Poster CSM32 □
2. Matteo Parente (DIFFER) - Photochemistry of metal@semiconductor core@shell nanostructures - Poster CSM36
3. Karthikeyan Gnanasekaran (TU/e) - Quantitative electron tomography of hierarchically assembled rod-like systems - Poster CSM18

### Room 63/64

1. Jurn Heinen (UvA) - Predicting Multicomponent Adsorption Isotherms in Open-Metal Site Materials using Density Functional Theory Derived Force Field Calculations - Poster ST26
2. Selim Sami (RUG) - Computation of dielectric constants of fullerene derivatives for organic photovoltaics - Poster ST20

### Room 65

1. Dina Petrova (UvA) - Microscopic visualisation of contacts and friction - Poster ST42
2. Sandra Wiersma (UvA) - Gas-phase infrared spectra of astronomical Polycyclic Aromatic Hydrocarbons measured with FELICE, the Free Electron Laser for Intra-Cavity Experiments - Poster ST
3. Gianluca Grimaldi (TUD) - Charge transfer in composite PbSe-CdSe NC films - Poster ST40

## Wednesday 7 December, 20.02 - 20.15

### room 55-57

1. Fleur van Beek (UvA) - Making Analytically Incompatible Approaches Compatible [Poster AC07](#)
2. Mengyun Xu (RUG) - A miniaturised protein microarray platform with quantification by internal calibration: Spot-to-spot correction [Poster AC53](#)

### Room 58

1. Sjors Wijnands (TU/e) - Controlling enzyme activity by modular protein recruitment on supramolecular polymers [Poster BMC61](#)
2. Liliana Cozzoli (RUG) - Controlling the self-assembly of DNA G-quadruplex micelles [Poster BMC11](#)
3. Shengqi Xiang (UU) - High sensitivity (1H)) solid-state NMR approaches applied to complex biomolecules [Poster AC55](#)

### Boszaal

1. Mira Holzheimer (RUG) - Asymmetric Total Synthesis of the Mycobacterial Glycolipid DAT2 [Poster DS13](#)
2. Pablo Ortiz (RUG) - Catalytic asymmetric alkylation of enolizable ketimines using Grignard reagents [Poster DS23](#)
3. Alejandra Riesco-Dominguez (RU) - Enantio- and diastereoselective synthesis of compound libraries based on the Piperidin-4-one scaffold [Poster DS27](#)

### Room 63/64

1. Tjerk Sminia (WUR) - Synthesis of Novel Probes for Metabolic Oligosaccharide Engineering in Bacteria [Poster DS31](#)
2. Andrea Leoncini (UT) - Influence of chirality, pre-organization and ionic liquids on the extraction of rare earths [Poster SR05](#)
3. Hidde Elferink (RU) - Stereoselective  $\beta$ -Mannosylation by Neighboring-Group Participation [Poster DS07](#)

### Parkzaal

1. Lara Vilarino Palmaz (RUG) - Supramolecular assembly of artificial metalloenzymes [Poster BMC55](#)
2. Xin Chen (RUG) - Investigating the peroxisomal membrane associated degradation (PMAD) pathway in yeast [Poster PR41](#)
3. Hanna Busch (TUD) - The re-evaluation and isolation of a novel Michael hydratase from Rhodococcus rhodochrous ATCC 17895 [Poster BMC05](#)

### Auditorium

1. Srividya Ganapathy (LEI) - Towards the adaptation of rhodopsin proton-pumps [Poster PR15](#)
2. Jan Pille (RU) - Self-assembling nanobodies for nanomedicine [Poster BMC45](#)
3. Patricia Alvarez Siero (RUG) - Formation of heterodimeric OpuA for smFRET studies [Poster Pr13](#)

### Room 82/83

1. Ingy Abdallah (RUG) - Amorphadiene Synthase: A Step Forward in Unraveling the Enigma of its Catalytic Mechanism [Poster PR01](#)
2. Cunliang Geng (UU) - Exploring the interplay between experimental methods and the performance of predictors of binding affinity change upon mutations in protein complexes [Poster PR33](#)

### Room 80/81

1. Can Araman (LEI) - Generation of citrullinated, bioorthogonal antigens to study their impact in rheumatoid arthritis [Poster BMC01](#)
2. Marcel van Willigen (UU) - A late assembly step can disrupt a well-folded domain in proteins [Poster PR57](#)
3. Luca Ferrari (UU) - Molecular chaperones stabilise protein oligomers linked to neurodegeneration [Poster PR55](#)

### Room 65

1. Clemens Mayer (RUG) - An epigenetics-inspired DNA-based data storage system [Poster NA05](#)

## Thursday 8 December, 9.05 - 9.25

### room 55-57

1. Guilia Lambiasi (VU) - Intact glycoform characterization of rHu EPO in HSA-containing formulations by HILIC-MS [Poster AC28](#)
2. Karlijn Bezemer (UvA) - Profiling of TATP using IRMS and GC-IRMS [Poster AC06](#)

### Boszaal

1. Pim de Vink (TU/e) - Multi-Component Assembly of an 14-3-3/Cucurbit[8]uril Supramolecular Protein Complex [Poster BMC56](#)
2. Selma Eising (RU) - A new bioorthogonal Carboni-Lindsey reaction with vinylboronic acids [Poster BMC16](#)
3. Dowine de Bruijn (RUG) - Bioorthogonal Metal Catalysis [Poster BMC02](#)

### Room 63/64

1. Mark Hoorens (UMCG) - Hemithioindigo photoswitches for biological applications [Poster MC18](#)
2. Marjolein Soethoudt (LEI) - Conformation-dependent labeling of the cannabinoid CB2 receptor for proof of target engagement in live cells [Poster MC34](#)
3. Xavier Gómez-Santacana (VU) - Photoisomerizable Phenylazo-Pyridines Enable the Control of Metabotropic Glutamate Receptor Subtype 5 Activity with Light [Poster MC10](#)

### Room 58

1. Ingrid 't Hart (UU) - Chemoenzymatic synthesis of Disialosyl Globopentaosylceramide (DSGb5) for cancer treatment [Poster MC14](#)
2. Raimond Heukers (VU) - Nanobody-mediated modulation of oncogenic properties of HCMV-encoded chemokine receptor US28 [Poster MC16](#)

### Parkzaal

1. Aleksandr Pogodaev (RU) - Light control of the enzymatic chemical reaction network [Poster BMC48](#)
2. Elliot Mock (LEI) - Mapping NAPE lipid signaling using photoaffinity labeling coupled with chemoproteomics [Poster MC26](#)
3. Alberto Juan Ruiz del Valle (UT) - NMR- STD highlights the binding site of a photo-switch based protein for simultaneous light-triggered ligand release [Poster BMC24](#)

### Auditorium

1. Hetty Manenschijn (Univ Geneva) - The contribution of myosin motors to membrane bending in endocytosis [Poster LB08](#)
2. Amin Abolghassemi Fakhree (UT) - The number of a-synuclein proteins per vesicle gives insights into its physiological function [Poster LB02](#)
3. Lukasz Syga (RUG) - Slow diffusion, steric exclusion and targeted protein delivery determine the localization of plasma membrane transporters - Poster LB12

### Room 82/83

1. Matti Pronker (UU) - Structural basis of the myelin-axon interaction [Poster PR62](#)
2. Doreth Kok (NKI) - DNA Mismatch repair - studying the activation states with cryo-EM [Poster PR50](#)

### Room 80/81

1. Hendrik Sikkema (RUG) - Elucidating the transport mechanism of the ABC-transporter OpuA: towards smFRET studies on OpuA in monodisperse nanoparticles [Poster PR24](#)
2. Emanuela Crisafi (LEI) - Investigating lipid interactions that control the molecular switch in photosynthetic light harvesting complex [Poster PR42](#)
3. Rajkumar Singh (RUG) - Biochemical and Structural characterization of NadR from L.Lactis in substrate bound and free conformation [Poster PR26](#)

### Room 65

1. Jeroen Strating (UU) - Viral hijacking of host cell membrane contact site machinery [Poster LB10](#)